



Biofilm growth in a homogeneous porous medium  
by Sunil Kumar Tiwari

A thesis submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in  
Mathematics

Montana State University

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Abstract:

As biofilms intervene in a porous medium, they affect the porosity and permeability, which in turn alters the hydrodynamics. A biofilm growth model is presented which is suitable for microscale simulations of biofilm activity in a porous medium. The model is then used to predict the changing porosity and permeability. The predictions are compared to experimental data and finally these calculated properties are used to simulate flow in a biofilm infested porous medium.

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This thesis has been read by each member of the thesis committee and has been found to be satisfactory regarding content, English usage, format, citations, bibliographic style, and consistency, and is ready for submission to the College of Graduate Studies.

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**ABSTRACT**

As biofilms intervene in a porous medium, they affect the porosity and permeability, which in turn alters the hydrodynamics. A biofilm growth model is presented which is suitable for microscale simulations of biofilm activity in a porous medium. The model is then used to predict the changing porosity and permeability. The predictions are compared to experimental data and finally these calculated properties are used to simulate flow in a biofilm infested porous medium.

## CHAPTER 1

# Introduction

The goal of this dissertation is to develop a mathematical model to describe the change in the hydrodynamic properties of a porous medium due to biofilm growth. A one-dimensional mathematical model called the Biofilm Growth Model (BGM) has been developed which describes the growth of biofilm on a surface. The results of the one-dimensional BGM and its zero-dimensional version have been compared. Also the results of the zero-dimensional BGM and the zero-dimensional versions of two existing models called the Biofilm Accumulation Model (BAM) and Rittman's model have been compared. Different model equations relating the porosity and the permeability of a porous medium have been discussed and some of the relations have been compared with the experimental data from [5], [6]. A complete porous media model describing the effect of biofilm growth on porosity, permeability, and hence the flow, has been presented. Finally, the numerical results of the one-dimensional porous media flow model simulations have been presented and these numerical results are compared with the experimental data from [5], [6].

Controlled, artificially grown biofilm in porous media provides significant opportunities for improving the performance of industrial and environmental processes. The petroleum industry, for example, uses biofilm for deliberate plugging of parts of the oil reservoir to enhance oil recovery. A controlled biofilm accumulation in high permeability zones can be used to prevent injection water from reaching the production well. This can be accomplished by injecting cells and nutrients into the oil-bearing formation, [16], [19]. Also, controlling biofilm accumulation is important

to both injection and production well operation in order to avoid unwanted formation plugging near the well bore. The environmental industry likewise uses deliberate plugging of pore channels between spilled contaminants and lakes or rivers to prevent the contamination of these water resources. Subsurface biofilms also offer the potential for biotransformation of organic compounds providing an in situ method (Figure 1) for treating contaminated groundwater supplies, [4], [26]. The mining industry is developing methods for microbially enhanced leaching of metals from ores and recovery of metals from solutions, [11]. An efficient use of biofilm by engineers

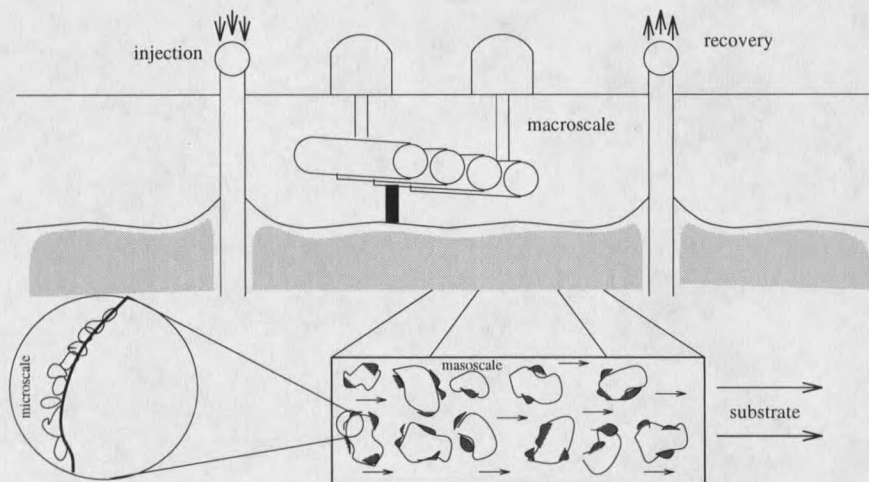


Figure 1: Injection/recovery scheme for enhancing in situ bioremediation of contaminated aquifer. Inset shows the growing biofilm in porous media.

requires an improved understanding of the interrelationship between porous media hydrodynamic properties and the accumulation rate and spatial distribution of the biofilm.

The pressure driven flow between two points in an isotropic homogeneous porous medium depends on the pressure gradient between the two points and the viscosity of the liquid flowing through it as well as the porosity and the permeability of the medium, [2], [7], [20]. If the pressure gradient between the two points and the viscosity of the liquid are assumed to be constant then the porosity and the

permeability dictate the flow rate. If one assumes the presence of an initial thin layer of biofilm on the pore surface and a high concentration of substrate (food for the bacteria) in the liquid flowing through the porous medium then it is reasonable to expect a decrease in the porosity and the permeability of the medium due to the biofilm growth in it. How fast does the biofilm grow? How does the flow rate change? In this work, a mathematical model has been developed that should help in the understanding of these issues.

In order to derive a mathematical model to study the effect of biofilm growth on porous media flow, one must combine the system of flow equations with a system of biofilm growth equations. A one-dimensional mathematical model called the Biofilm Growth Model (BGM) has been developed in Chapter 2 which describes the growth of a biofilm on a surface. The one-dimensional Biofilm Accumulation Model (BAM, [14], originally developed in [25]) and Rittman's model (originally developed in [12]) have also been described in Chapter 2. Based on Rittman's zero-dimensional model, the zero-dimensional versions of BAM and BGM have also been derived. A zero-dimensional model ignores the spatial dependence of the variables, namely the substrate concentration in the biofilm and the volume fraction of the active and inactive bacteria in the biofilm and describes the change in the spatial average value of these variables with respect to time.

A comparison, undertaken in Chapter 3, of the numerical solutions of one-dimensional BGM and zero-dimensional BGM show that (i) the qualitative behavior of the solutions from both the models are very similar and they are also quantitatively close, and (ii) the zero-dimensional model equations are comparatively easy to solve and the computation time is much less than the computation time for the one-dimensional model. The zero-dimensional model lacks some of the features which the one-dimensional model possesses. For example, the substrate concentration or the

active biomass volume fraction at a certain point in the biofilm can not be computed with a zero-dimensional model. However, since we intend to use the biofilm growth model in a porous medium setting, the zero-dimensional BGM is chosen over the one-dimensional BGM. This is because the zero-dimensional model efficiently describes the average change in the substrate concentration and the biofilm thickness which suffices our need. After a comparison of the three zero-dimensional models (BGM, BAM, and Rittman's model), also completed in Chapter 3, the zero-dimensional BGM has been chosen over the other two models primarily because BGM assumes the bulk volume (in the case of a porous medium it is the pore volume) to be a variable as opposed to the other two models (BAM and Rittman's model) in which the bulk volume is assumed to be a constant. This is necessary in order to study the effect of biofilm growth on porosity and hence permeability.

The relation between porosity and permeability of a porous medium has been investigated by many researchers in the past. A collection of experiment-based algebraic relations between porosity and permeability and a list of references can be found in the Chapter 3 of [9]. Some of the relations which are relevant for the models developed in this dissertation are described here in Chapter 4 and the validity of two of such formulas has been checked against the experimental data given in [5], [6]. Finally in Chapter 4, the complete model describing biofilm growth in a porous medium and its effect on porosity and the permeability of the medium is formulated.

The complete model describing the biofilm growth in a homogeneous porous medium and its effect on the one-dimensional incompressible fluid flow through the medium is numerically solved in Chapter 5 and numerical solutions are presented. The model equations are solved for a short bed (5 cm long) of spherical balls and a long bed (60 cm long) of spherical balls. The numerical results for a short bed experiment have been compared with the experimental data from [5], [6]. Lastly, the

change in the variables over time is predicted for a long bed experiment.

## CHAPTER 2

**Biofilm Models****Introduction**

What follows is the discussion of biofilm growth on a surface. In addition, the derivation of one-dimensional and zero-dimensional mathematical models which describe these physical phenomena is given.

Consider a water filled tank with an initial biofilm thickness on one of its walls. Assume that the substrate (food or nutrient) for the bacteria is dissolved in the water and diffuses into the biofilm. The bacteria in the biofilm will consume the substrate and will multiply. The growth of the biofilm (increase in thickness) depends on the volume fraction of the active biomass, the substrate concentration in the biofilm, the substrate concentration in the bulk liquid in the tank, the rate of the consumption of the substrate by the bacteria, the diffusion rate of the substrate in the biofilm, and possibly other factors. In fact, the growth of the biofilm is a very complicated phenomenon and to produce an accurate mathematical model is not easy. This physical system is shown in Figure 2, where  $L(t)$  is the biofilm thickness at time  $t$ ,  $u(L, t)$  is the biomass velocity at the film-water interface and  $Q$  is the volumetric flow rate of the influent fluid.

A similar problem has been discussed in [12] and [25] and one-dimensional models have been derived that describe the growth of the thickness of a biofilm with respect to time and space. The model developed in [12] is also called **Rittman's**

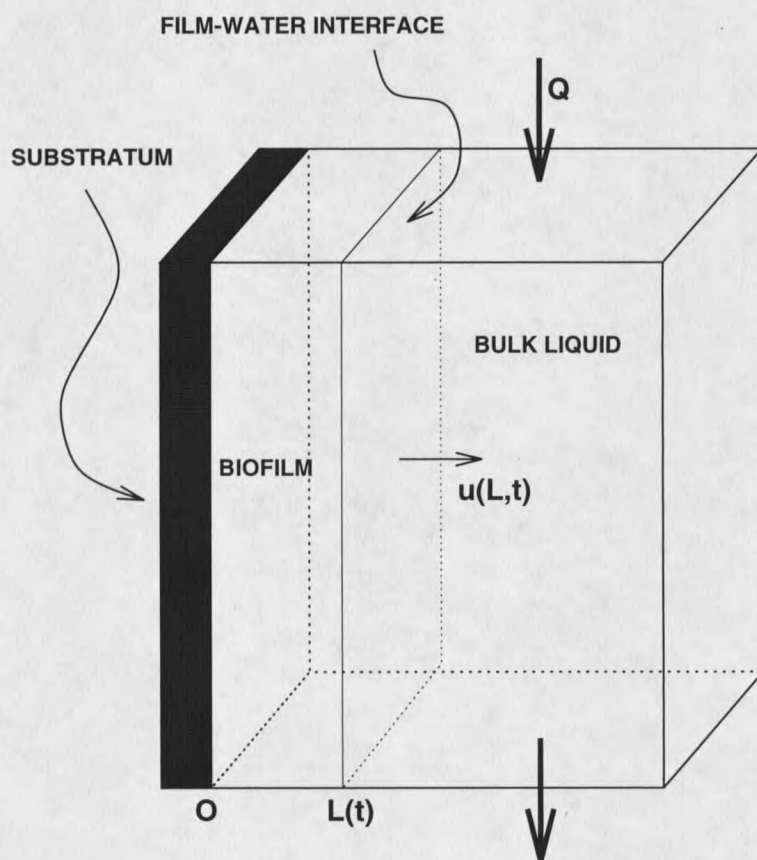


Figure 2: Biofilm on a surface

**Model.** The Center for Biofilm Engineering at Montana State University, has developed a computer simulator called the **Biofilm Accumulation Model, (BAM)**, [14] which studies the growth of biofilm on a flat surface. The model equations are based on [25]. Both of these models assume the volume of the bulk liquid is constant. Also some of the terms in the model equations are not consistent with the underlying assumptions. Hence a new model called the **Biofilm Growth Model (BGM)** is developed here which considers the volume of the bulk liquid to be a time-dependent function instead of a constant. The equations described in these models cannot be used directly in a problem where biofilm grows in a porous media because of the simplified assumptions of these models and the complicated geometry of the pore surface, however the idea of the zero-dimensional model discussed in [12] is very useful here. In both Rittman's model and BAM, different types of bacteria are consuming different types of substrates and are growing simultaneously. But, for now, in order to keep the notation clean and the problem simple and explainable, we shall restrict ourselves to only one bacteria consuming only one substrate.

## Rittman's Model

### One-dimensional Model

In this model, originally proposed in [12], the microbial interactions and diffusion phenomena are described by two sets of mathematical equations. The first set is called diffusional equations, the other one transport equations. They are derived from basic mass balances. The following *a priori* assumptions have been made to develop this model:

- The biofilm is homogeneous and can be treated as a continuum.
- Changes occur only in the direction normal to the biofilm surface.

- There is a laminar diffusional sublayer of constant thickness in the bulk liquid.
- The biofilm is composed entirely of active or inactive biomass.

This model predicts four time-dependent functions, two of which depend on the spatial variable  $y$  as well. These functions and their fundamental units of length ( $L$ ) and substrate mass ( $M_s$ ) are given in Table 1.

Variables	Physical quantity	Units
$L(t)$	biofilm thickness	$L$
$S_b(t)$	bulk substrate concentration	$M_s L^{-3}$
$S(y, t)$	substrate concentration in the biofilm	$M_s L^{-3}$
$f(y, t)$	volume fraction of active biomass in the biofilm	dimensionless

Table 1: Unknown dependent variables and their fundamental units in Rittman's one-dimensional model

Other variables and the parameters used in the development of this model and their fundamental units of length ( $L$ ), time ( $T$ ), substrate mass ( $M_s$ ), and biomass ( $M_x$ ), are given in Table 2.

A visualization of the physical system to be modeled is given in Figure 3 where  $\sigma$  is the surface area of the film-water interface.

**Diffusional Equations** The mass balance equation for the total substrate in the bulk liquid,  $V_L S_b$ , has the form

$$V_L \frac{d}{dt}(S_b(t)) = Q(S_0 - S_b(t)) - \sigma J(t), \quad (2.1)$$

where  $V_L$  is the volume ( $L^3$ ),  $Q$  represents the bulk liquid flow rate ( $L^3 T^{-1}$ ),  $\sigma$  is the surface area of the film-water interface ( $L^2$ ),  $S_0$  refers to the influent substrate concentration ( $M_s L^{-3}$ ) and  $J(t)$  refers to the substrate flux through the laminar diffusional sublayer ( $M_s L^{-2} T^{-1}$ ).  $V_L, Q, \sigma$  and  $S_0$  are assumed constant. According

Parameters	Physical quantity	Units
$V_L$	volume of the bulk liquid	$L^3$
$Q$	volumetric flow rate of the bulk liquid	$L^3T^{-1}$
$S_0$	substrate concentration in the influent fluid	$M_sL^{-3}$
$\sigma$	area of the film-water interface	$L^2$
$D$	diffusivity coefficient of the substrate through the laminar diffusional sublayer	$L^2T^{-1}$
$L_l$	thickness of laminar diffusional sublayer	$L$
$d$	diffusivity coefficient of the substrate inside the biofilm	$L^2T^{-1}$
$V_r$	maximum specific growth rate	$M_sM_x^{-1}T^{-1}$
$K$	Monod constant	$M_sL^{-3}$
$\rho$	biomass density	$M_xL^{-3}$
$b$	inactivation coefficient of bacteria	$T^{-1}$
$Y$	yield coefficient	$M_xM_s^{-1}$
$G_s$	global shear stress coefficient	$T$
$B'$	average shear stress coefficient	$T^{-1}$
$f_d$	biodegradable fraction of the biomass	dimensionless
Variables	Physical quantity	Units
$J(t)$	influx rate of the substrate into the biofilm	$M_sL^{-2}T^{-1}$
$u(y, t)$	velocity of the biomass particle at $(y, t)$	$LT^{-1}$
$G(y, t)$	active biomass quantity in the interval $[0, y]$	$M_xL^{-2}$
$c(y, t)$	net growth of active biomass	$M_xL^{-3}T^{-1}$
$R(y, t)$	reaction rate	$M_sL^{-3}T^{-1}$
$b'(y)$	shear function along y-axis	$T^{-1}$
$f_0(t)$	volume fraction at the substratum	dimensionless
$\bar{G}(y, t)$	inactive biomass quantity in the interval $[0, y]$	$M_xL^{-2}$
$\bar{f}(y, t)$	volume fraction of inactive biomass in the biofilm	dimensionless
$\bar{c}(y, t)$	net growth of inactive biomass	$M_xL^{-3}T^{-1}$
$B(y, t)$	total biomass amount	$M_xL^{-2}$

Table 2: Parameters and the variables used in Rittman's model and their fundamental units

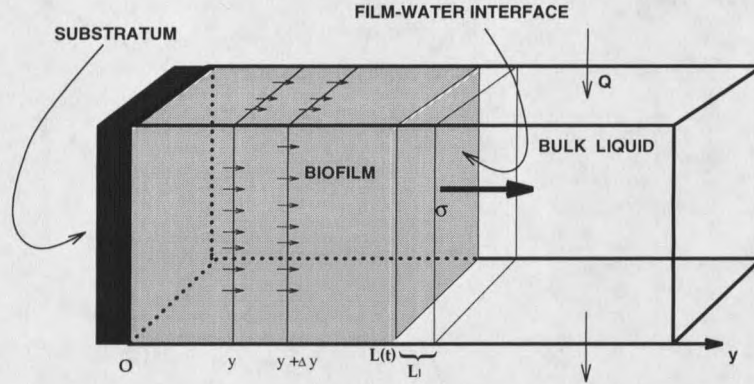


Figure 3: Biofilm on a surface

to Fick's first law,  $J(t)$  is expressed by

$$J(t) = \frac{D}{L_l} \left( S_b(t) - S(L(t), t) \right), \quad (2.2)$$

where  $D$  is the diffusivity coefficient of the substrate through the laminar diffusional sublayer ( $L^2T^{-1}$ ) and  $L_l$  is the thickness of the laminar diffusional sublayer ( $L$ ). Both  $D$  and  $L_l$  are constants. Combining (2.1) and (2.2) yields

$$\frac{d}{dt}(S_b(t)) = \frac{1}{V_L} \left( Q S_0 - \left( Q + \frac{\sigma D}{L_l} \right) S_b(t) + \frac{\sigma D}{L_l} S(L(t), t) \right). \quad (2.3)$$

The mass balance on the substrate in the biofilm ( $0 \leq y \leq L(t)$ ) is expressed by

$$\frac{\partial S(y, t)}{\partial t} = d \frac{\partial^2 S(y, t)}{\partial y^2} - R(y, t), \quad (2.4)$$

where  $d$  is the constant diffusivity coefficient of the substrate inside the biofilm ( $L^2T^{-1}$ ). The reactional term,  $R(y, t)$ , which is based on Monod kinetics [10] and is given as

$$R(y, t) = R(S(y, t), f(y, t)) = \frac{V_r S(y, t)}{K + S(y, t)} f(y, t) \rho. \quad (2.5)$$

Here  $V_r$  represents the maximum specific growth rate ( $M_s M_x^{-1} T^{-1}$ ),  $K$  represents the Monod coefficient ( $M_s L^{-3}$ ), and  $\rho$  is the biomass density ( $M_x L^{-3}$ ) where  $M_x$  is the

fundamental unit of biofilm mass.  $V_r, \rho$ , and  $K$  are all assumed constant. Combining (2.4) and (2.5) gives

$$\frac{\partial S(y, t)}{\partial t} = d \frac{\partial^2 S(y, t)}{\partial y^2} - \frac{V_r S(y, t)}{K + S(y, t)} f(y, t) \rho. \quad (2.6)$$

The boundary conditions state that there is no substrate flux through the substratum ( $y = 0$ ), and at the film-water interface ( $y = L(t)$ ) the flux through the biofilm is equal to the flux through the laminar diffusional sublayer. Hence,

$$-d \frac{\partial S}{\partial y}(0, t) = 0, \quad (2.7)$$

and

$$-d \frac{\partial S}{\partial y}(L(t), t) = -J(t). \quad (2.8)$$

The differential equations (2.3) and (2.6) and the boundary conditions (2.7) and (2.8) are the diffusional set of equations for Rittman's model.

**Transport Equations** To describe biomass growth we define a control volume which has surface area  $\sigma$  and extends from  $y = 0$  to  $y = y(t)$  with  $y(t) \leq L(t)$ . At time  $t + dt$  this volume has grown and the control volume extends from  $y = 0$  to  $y = y(t + dt)$ .

The biomass particle speed  $u(y, t)$ , ( $LT^{-1}$ ), is described by  $u(t) = \frac{dy}{dt}$ . The active biomass quantity  $G(y, t)$ , ( $M_x L^{-2}$ ), on the interval  $[0, y]$  is expressed by

$$G(y, t) = \int_0^y \rho f(\xi, t) d\xi. \quad (2.9)$$

Since the interval  $[0, y(t)]$  at time  $t$  grows to the interval  $[0, y(t + dt)]$  at time  $t + dt$  we can let  $dt \rightarrow 0$  and obtain the time derivative of  $G(y, t)$ , which is a particle time derivative, given by

$$\lim_{dt \rightarrow 0} \frac{G(y(t + dt), t + dt) - G(y(t), t)}{dt} = \frac{d}{dt}(G(y(t), t)) = u \frac{\partial G}{\partial y} + \frac{\partial G}{\partial t}. \quad (2.10)$$

Then an active biomass balance may be written. The time rate of change of  $G(y, t)$  is equal to the sum of the growth of active biomass minus the biomass lost by shear stress. Thus

$$u(y, t) \frac{\partial G}{\partial y} + \frac{\partial G}{\partial t} = \int_0^y \left( c(\xi, t) - b'(\xi) f(\xi, t) \rho \right) d\xi; \quad (2.11)$$

where  $c(y, t)$  is the net growth of active biomass ( $M_x L^{-3} T^{-1}$ ), which results from a production term minus a decay term. The net growth  $c(y, t)$  is expressed as

$$c(y, t) = YR(S(y, t), f(y, t)) - bf(y, t)\rho \quad (2.12)$$

where  $Y$  is the yield coefficient ( $M_x M_s^{-1}$ ),  $b$  represents the inactivation coefficient of bacteria ( $T^{-1}$ ) and  $b'(y)$  is a shear function along the  $y$ -axis ( $T^{-1}$ ). Both  $Y$  and  $b$  are assumed constant. Shear stress is expressed as a function of spatial and temporal variables  $y$  and  $t$  rather than as a constant applied only at the biofilm surface, avoiding the Dirac effect of discontinuity. That is why this term appears inside the integral and is not simply added at the biofilm surface. The shear function  $b'(y)$  used for this work is

$$b'(y) = \frac{1 + \arctan(30(y - .9))}{.2G_s}, \quad (2.13)$$

where the detachment layer thickness is fixed at 20% of the biofilm thickness.  $G_s$  is an experimental constant which represents a fraction of biomass detached from total biomass ( $T$ ). The shear function  $b'(y)$  describes biomass loss distributed throughout the biofilm and a detachment layer is defined everywhere  $b'(y) > 0$ . Taking the partial derivative of (2.11) with respect to  $y$ , using the definition of  $G(y, t)$  from (2.9) and dividing by  $\rho$ , which is a constant, yields

$$\frac{\partial f(y, t)}{\partial t} + u(y, t) \frac{\partial f(y, t)}{\partial y} = \frac{c(y, t)}{\rho} - b'(y) f(y, t) - f(y, t) \frac{\partial u}{\partial y}. \quad (2.14)$$

As biomass growth does not occur at the substratum we introduce the following boundary conditions

$$f(0, t) = f_0(t) \quad (2.15)$$

$$\begin{aligned} \frac{df_0}{dt} = & \left( Y \frac{V_r S(0, t)}{K + S(0, t)} - b \right) f_0(t) \\ & - f_0(t) \frac{\partial u}{\partial y}(0, t) \end{aligned} \quad (2.16)$$

where  $f_0(t)$  is the dimensionless volume fraction at the substratum ( $y = 0$ ). Similar to the above treatment of the active biomass quantities,  $G(y, t)$ , we can introduce the inert biomass amount  $\bar{G}(y, t)$ , ( $M_x L^{-2}$ ), on the interval  $[0, y]$ . It can be expressed by

$$\bar{G}(y, t) = \int_0^y \rho \bar{f}(\xi, t) d\xi, \quad (2.17)$$

where  $\bar{f}(y, t)$  is the volume fraction of the inert biomass. The inert biomass balance is then given as

$$u(y, t) \frac{\partial \bar{G}}{\partial y} + \frac{\partial \bar{G}}{\partial t} = \int_0^y \left( \bar{c}(\xi, t) - b'(\xi) \rho \bar{f}(\xi, t) \right) d\xi, \quad (2.18)$$

where  $\bar{c}(y, t)$  is the net inert biomass increase ( $M_x L^{-3} T^{-1}$ ). This function is given as

$$\bar{c}(y, t) = b(1 - f_d) f(y, t) \rho \quad (2.19)$$

where  $f_d$  is the dimensionless biodegradable fraction of biomass, which is a constant between 0 and 1. We can now express the total biomass amount  $B(y, t)$  on interval  $[0, y]$  as

$$B(y, t) = G(y, t) + \bar{G}(y, t) = \int_0^y \rho \left( \bar{f}(\xi, t) + f(\xi, t) \right) d\xi = y \rho \quad (2.20)$$

because  $\bar{f}(y, t) + f(y, t) = 1$ . Hence  $B(y, t)$  is independent of  $t$ . Adding (2.11) and (2.18) we can express the particle derivative of  $B(y, t)$  as

$$\begin{aligned} u(y, t) \frac{\partial B}{\partial y} + \frac{\partial B}{\partial t} = & \int_0^y \left( \left( \bar{c}(\xi, t) + c(\xi, t) \right) \right. \\ & \left. - b'(\xi) \rho \left( \bar{f}(\xi, t) + f(\xi, t) \right) \right) d\xi. \end{aligned} \quad (2.21)$$

Using (2.20) this reduces to

$$u(y, t) \rho = \int_0^y \left( \left( \bar{c}(\xi, t) + c(\xi, t) \right) - b'(\xi) \rho \left( \bar{f}(\xi, t) + f(\xi, t) \right) \right) d\xi \quad (2.22)$$

which simplifies to

$$u(y, t) = \int_0^y \left( \frac{Y}{\rho} R(S(\xi, t), f(\xi, t)) - b f_a f(\xi, t) - b'(\xi) \right) d\xi. \quad (2.23)$$

Hence, the velocity of the film-water interface will be given by,

$$u(L(t), t) = \frac{dL(t)}{dt} = \int_0^{L(t)} \left( \frac{Y}{\rho} R(S(\xi, t), f(\xi, t)) - b f_a f(\xi, t) - b'(\xi) \right) d\xi. \quad (2.24)$$

Equations (2.14), (2.23), and (2.24) and the boundary conditions (2.15), (2.16) are referred to as the transport equations.

### One-dimensional Rittman's Model

#### Diffusional Equations $0 \leq y \leq L(t)$

$$\frac{d}{dt}(S_b(t)) = \frac{1}{V_L} \left( Q S_0 - \left( Q + \frac{\sigma D}{L_l} \right) S_b(t) + \frac{\sigma D}{L_l} S(L(t), t) \right) \quad (2.25)$$

$$\frac{\partial S(y, t)}{\partial t} = d \frac{\partial^2 S(y, t)}{\partial y^2} - \frac{V_r S(y, t)}{K + S(y, t)} f(y, t) \rho \quad (2.26)$$

#### Boundary Conditions

$$-d \frac{\partial S}{\partial y}(0, t) = 0 \quad (2.27)$$

$$-d \frac{\partial S}{\partial y}(L(t), t) = -\frac{D}{L_l} \left( S_b(t) - S(L(t), t) \right) \quad (2.28)$$

#### Transport Equations $0 \leq y \leq L(t)$

$$\begin{aligned} \frac{\partial f(y, t)}{\partial t} + u(y, t) \frac{\partial f(y, t)}{\partial y} &= \left( Y \frac{V_r S(y, t)}{K + S(y, t)} - b \right. \\ &\quad \left. - b'(y) \right) f(y, t) - f(y, t) \frac{\partial u(y, t)}{\partial y} \end{aligned} \quad (2.29)$$

$$u(y, t) = \int_0^y \left( \left( Y \frac{V_r S(\xi, t)}{K + S(\xi, t)} - b f_d \right) f(\xi, t) - b'(\xi) \right) d\xi \quad (2.30)$$

Boundary Conditions

$$f(0, t) = f_0(t) \quad (2.31)$$

$$\begin{aligned} \frac{df_0}{dt} &= \left( Y \frac{V_r S(0, t)}{K + S(0, t)} - b \right) f_0(t) \\ &\quad - f_0(t) \frac{\partial u}{\partial y}(0, t) \end{aligned} \quad (2.32)$$

$$\frac{dL(t)}{dt} = u(L(t), t) \quad (2.33)$$

### Zero-dimensional Model

In the model described above, the functions  $S(y, t)$  and  $f(y, t)$  depend on time as well as space. The zero-dimensional model ignores the dependence of these functions on the spatial variable  $y$  and considers the average growth and decay of the functions  $S$  and  $f$  on the interval  $0 \leq y \leq L(t)$ , which depend on time only. The four dependent variables and their fundamental units are given in Table 1. A detailed description and derivation of the zero-dimensional equations follows.

Variables	Physical quantity	Units
$L(t)$	biofilm thickness	$L$
$S_b(t)$	bulk substrate concentration	$M_s L^{-3}$
$S(t)$	average substrate concentration in the biofilm	$M_s L^{-3}$
$f(t)$	average volume fraction of active biomass in the biofilm	dimensionless

Table 3: Unknown dependent variables and their fundamental units in Rittman's zero-dimensional model

The derivation follows along the same lines as that for the one-dimensional model. Let  $S(t)$  be the average value of  $S(y, t)$  for  $y \in [0, L(t)]$  and let  $f(t)$  be the average value of  $f(y, t)$  for  $y \in [0, L(t)]$ . A substrate balance in the bulk fluid gives

(see (2.1)),

$$V_L \frac{d}{dt}(S_b(t)) = Q(S_0 - S_b(t)) - \sigma J(t) \quad (2.34)$$

where

$$J(t) = \frac{D}{L_l}(S_b(t) - S(t)).$$

Hence (2.34) simplifies to the zero-dimensional version of (2.3)

$$\frac{d}{dt}(S_b(t)) = \frac{1}{V_L} \left( Q S_0 - \left( Q + \frac{\sigma D}{L_l} \right) S_b(t) + \frac{\sigma D}{L_l} S(t) \right). \quad (2.35)$$

The mass balance of the substrate in the biofilm is given by (see (2.6))

$$\frac{d}{dt}(L(t)S(t)) = \frac{D}{L_l}(S_b(t) - S(t)) - \frac{V_r S(t)}{K + S(t)} L(t) f(t) \rho, \quad (2.36)$$

where the first term on the right-hand side is the rate of diffusion of the substrate from the bulk fluid to the laminar diffusional sublayer of thickness  $L_l$  of the biofilm and the second term is the average consumption rate of the substrate by the species based on Monod kinetics. This is the zero-dimensional version of (2.6). The mass balance of the active biomass in the biofilm is

$$\begin{aligned} \text{rate of increase of the active biomass} &= \text{growth rate due to} \\ &\quad \text{substrate consumption} \\ &\quad - \text{rate of cell decay} \\ &\quad - \text{detachment rate} \end{aligned}$$

which translates into (see (2.14))

$$\frac{d}{dt}(L(t)f(t)\rho) = \left( Y \frac{V_r S(t)}{K + S(t)} - (b + B') \right) L(t)f(t)\rho$$

where  $B'$  is the average shear stress coefficient (average value of  $b'$  for  $y \in [0, L(t)]$ ).

Dividing by  $\rho$  yields the zero-dimensional version of (2.14)

$$\frac{d}{dt}(L(t)f(t)) = \left( Y \frac{V_r S(t)}{K + S(t)} - (b + B') \right) L(t)f(t). \quad (2.37)$$

Similarly, the mass balance of the inactive biomass in the biofilm is

$$\begin{aligned} \text{rate of increase of the inactive biomass} &= \text{inactivation rate} \\ &\quad \text{of active bacteria} \\ &\quad - \text{bio-degradation rate} \\ &\quad - \text{detachment rate} \end{aligned}$$

which translates into

$$\frac{d}{dt}(L(t)\bar{f}(t)\rho) = bL(t)f(t)\rho - bf_dL(t)f(t)\rho - B'L(t)\bar{f}(t)\rho.$$

Dividing by  $\rho$ , adding with (2.37), and using the assumption  $f(t) + \bar{f}(t) = 1$  yields

$$\frac{d}{dt}(L(t)) = \left( Y \frac{V_r S(t)}{K + S(t)} - bf_d \right) L(t)f(t) - B'L(t), \quad (2.38)$$

which is the zero-dimensional version of (2.30). Again  $B'$  is the average shear stress coefficient ( $T^{-1}$ ).

### Zero-dimensional Rittman's Model

$$\frac{d}{dt}(S_b(t)) = \frac{1}{V_L} \left( QS_0 - \left( Q + \frac{\sigma D}{L_l} \right) S_b(t) + \frac{\sigma D}{L_l} S(t) \right) \quad (2.39)$$

$$\frac{d}{dt}(L(t)S(t)) = \frac{D}{L_l} (S_b(t) - S(t)) - \frac{V_r S(t)}{K + S(t)} L(t)f(t)\rho \quad (2.40)$$

$$\frac{d}{dt}(L(t)f(t)) = \left( Y \frac{V_r S(t)}{K + S(t)} - (b + B') \right) L(t)f(t) \quad (2.41)$$

$$\frac{d}{dt}(L(t)) = \left( Y \frac{V_r S(t)}{K + S(t)} - bf_d \right) L(t)f(t) - B'L(t) \quad (2.42)$$

## Biofilm Accumulation Model

### One-dimensional Model

In this model, originally described in [25], the mathematical description of microbial interaction in a fixed biofilm is based on conservation principles. This model has the same underlying assumptions as that of Rittman's model hence the mathematical model equations are similar. But when it comes to modeling the detachment of the biofilm into the bulk liquid, these two models differ. Since detachment occurs only at the film-water interface, BAM assumes the effect of detachment close to the interface only whereas Rittman's model assumes that the detachment effects all the variables at each spatial point.

It is assumed that

- The biofilm is homogeneous and may be treated as a continuum.
- The changes occur only in the direction perpendicular to the biofilm surface.
- There is a laminar diffusional sublayer of constant thickness in the bulk liquid.
- The biofilm is made of active and inactive cells of bacteria and water.

This model will predict the same four functions as in Table 1. The other variables and different parameters used to develop this model along with their fundamental units are given in Table 4. A visualization of the physical system to be modeled is given in Figure 4

This model also consists of two sets of differential equations. One is the diffusional equations and the other is the transport equations.

Diffusional Equations The mass balance of substrate is given by,

$$\frac{\partial}{\partial t}(S(y, t)) = \left( -R(y, t) - \frac{\partial J(y, t)}{\partial y} \right) \quad (2.43)$$

Parameters	Physical quantity	Units
$V_L$	volume of the bulk liquid	$L^3$
$\epsilon_l$	volume fraction of water in the biofilm	dimensionless
$Q$	volumetric flow rate of the bulk liquid	$L^3T^{-1}$
$S_0$	substrate concentration in the influent fluid	$M_sL^{-3}$
$\sigma$	area of the film-water interface	$L^2$
$D$	diffusivity coefficient of the substrate through the laminar diffusional sublayer	$L^2T^{-1}$
$L_l$	thickness of laminar diffusional sublayer	$L$
$d$	diffusivity coefficient of the substrate inside the biofilm	$L^2T^{-1}$
$\rho$	biomass density	$M_xL^{-3}$
$b$	inactivation coefficient	$T^{-1}$
$Y$	yield coefficient	$M_xM_s^{-1}$
$\lambda$	detachment coefficient	$L^{-1}T^{-1}$
Variables	Physical quantity	Units
$J(y,t)$	influx rate of the substrate into the biofilm	$M_sL^{-2}T^{-1}$
$u(y,t)$	velocity of the biomass particle at $(y,t)$	$LT^{-1}$
$u_L(t)$	velocity of the film-water interface	$LT^{-1}$
$g(y,t)$	flux of active biomass	$M_xL^{-2}T^{-1}$
$R(y,t)$	reaction rate	$M_sL^{-3}T^{-1}$
$\delta(t)$	detachment rate of the biofilm	$LT^{-1}$
$\bar{f}(y,t)$	volume fraction of inactive biomass in the biofilm	dimensionless

Table 4: Parameters and the variables used in BAM and their fundamental units

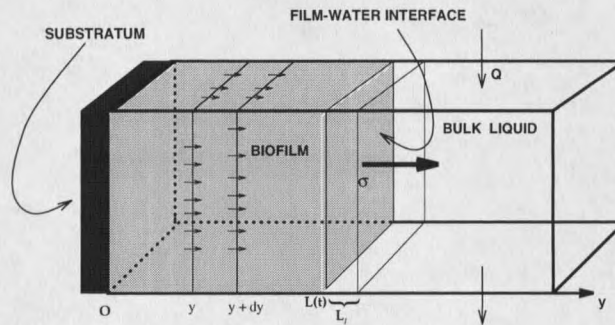


Figure 4: Biofilm on a surface

where  $S(y, t)$  is the concentration of the substrate in the biofilm ( $M_s L^{-3}$ ),  $J(y, t)$  is the flux of substrate into the biofilm, ( $M_s L^{-2} T^{-1}$ ), and  $R(y, t)$  is the reaction rate of substrate, ( $M_s L^{-3} T^{-1}$ ).

According to Fick's first law, the flux of substrate within the film is proportional to the diffusivity  $d$  ( $L^2 T^{-1}$ ) and may be expressed as

$$J(y, t) = -d \frac{\partial S(y, t)}{\partial y}. \quad (2.44)$$

Substitution of equation (2.44) into equation (2.43) leads to

$$\frac{\partial S(y, t)}{\partial t} = \left( -R(y, t) + \frac{\partial}{\partial y} \left( d \frac{\partial S(y, t)}{\partial y} \right) \right). \quad (2.45)$$

At the substratum there is no flux which gives

$$\frac{\partial S}{\partial y}(0, t) = 0. \quad (2.46)$$

If an external mass transfer limitation is included, then the other boundary condition at the film-water interface is

$$d \frac{\partial S}{\partial y}(L(t), t) = \frac{D}{L_l} \left( S_b(t) - S(L(t), t) \right) \quad (2.47)$$

and if it is neglected then,

$$S_b(t) = S(L(t), t), \quad (2.48)$$

where  $D$  is the diffusivity of the substrate in the laminar diffusional sublayer ( $L^2 T^{-1}$ ),  $L_l$  is the thickness of the laminar sublayer ( $L$ ), and  $S_b(t)$  is the concentration of the substrate in the bulk liquid.  $D$  and  $L_l$  are assumed to be constants.

Finally the model equation for the substrate in the bulk liquid is

$$\frac{dS_b(t)}{dt} = \frac{1}{V_L} \left( Q \left( S_0 - S_b(t) \right) - \sigma \left( \frac{D}{L_l} - u(L(t), t) \right) \left( S_b(t) - S(L(t), t) \right) \right). \quad (2.49)$$

The differential equations (2.45) and (2.49) and the boundary conditions (2.46) and (2.47) are the diffusional equations for BAM.

**Transport Equations** A mass balance of active microbial species for a differential volume  $\sigma dy$ , as shown in Figure 4, has the form

$$\begin{aligned} \frac{\partial}{\partial t} \left( \sigma dy \rho f(y, t) \right) &= \sigma dy Y R(y, t) - b \sigma dy \rho f(y, t) \\ &+ \sigma g(y, t) - \sigma g(y + dy, t), \end{aligned} \quad (2.50)$$

where  $\sigma$  is the area of the film-water interface ( $L^2$ ),  $\sigma dy$  is the differential volume element ( $L^3$ ),  $\rho$  is the constant density of the biomass ( $M_x L^{-3}$ ),  $R(y, t)$  is the reaction rate of the active biomass ( $M_s L^{-3} T^{-1}$ ),  $f(y, t)$  is the dimensionless volume fraction of the active biomass,  $b$  is the inactivation coefficient ( $T^{-1}$ ), and  $g(y, t)$  is the mass flux ( $M_x L^{-2} T^{-1}$ ). Approximating  $g(y + dy, t)$  by its first-order Taylor's expansion, (2.50) reduces to

$$\frac{\partial}{\partial t} \left( \sigma dy \rho f(y, t) \right) = \sigma dy Y R(y, t) - b \sigma dy \rho f(y, t) - \sigma \frac{\partial g(y, t)}{\partial y} dy. \quad (2.51)$$

Dividing by  $\sigma dy \rho$  we get,

$$\frac{\partial f(y, t)}{\partial t} = \frac{Y}{\rho} R(y, t) - b f(y, t) - \frac{1}{\rho} \frac{\partial g(y, t)}{\partial y}. \quad (2.52)$$

The flux  $g(y, t)$  of active biomass may be expressed in terms of the velocity  $u(y, t)$  at which the microbial mass is displaced with respect to the substratum and the concentration of the microorganisms  $\rho f(y, t)$ , as

$$g(y, t) = u(y, t) \rho f(y, t). \quad (2.53)$$

Now (2.52) implies,

$$\frac{\partial f(y, t)}{\partial t} = \frac{Y}{\rho} R(y, t) - b f(y, t) - \frac{\partial u(y, t)}{\partial y} f(y, t) - u(y, t) \frac{\partial f(y, t)}{\partial y}. \quad (2.54)$$

Similarly the mass balance of the inactive biomass simplifies to

$$\frac{\partial \bar{f}(y, t)}{\partial t} = b f(y, t) - \frac{\partial u(y, t)}{\partial y} \bar{f}(y, t) - u(y, t) \frac{\partial \bar{f}(y, t)}{\partial y} \quad (2.55)$$

where  $\bar{f}(y, t)$  is the dimensionless volume fraction of inactive biomass. Adding (2.54) and (2.55) and assuming that  $f(y, t) + \bar{f}(y, t) = 1 - \epsilon_l$ , where  $\epsilon_l$  is the constant dimensionless volume fraction of water in the biofilm, we get

$$0 = \frac{Y R(y, t)}{\rho} - (1 - \epsilon_l) \frac{\partial u(y, t)}{\partial y} \quad (2.56)$$

which simplifies to

$$\frac{\partial u(y, t)}{\partial y} = \frac{1}{(1 - \epsilon_l)} \frac{Y R(y, t)}{\rho}. \quad (2.57)$$

Integrating both sides and using the assumption that  $u(0, t) = 0$  we get

$$u(y, t) = \frac{1}{(1 - \epsilon_l)} \int_0^y \frac{Y R(\xi, t)}{\rho} d\xi. \quad (2.58)$$

If the biofilm grows or shrinks, the thickness  $L(t)$  of the biofilm changes and the film-water interface moves at a velocity

$$u_L(t) \equiv u(L(t), t) = \frac{dL(t)}{dt} \quad (2.59)$$

with respect to the substratum. If  $\delta(t)$  is defined to be the velocity ( $LT^{-1}$ ), at which biomass is exchanged between biofilm and the bulk liquid (detachment rate), then using equation (2.58) the velocity of the film-water interface may be expressed as

$$u_L(t) = \frac{1}{(1 - \epsilon_l)} \int_0^{L(t)} \frac{Y R(\xi, t)}{\rho} d\xi + \delta(t). \quad (2.60)$$

The detachment function,  $\delta(t)$ , is given by  $\delta(t) = -\lambda L^2(t)$ , [25]. The constant  $\lambda$  is called the coefficient of detachment ( $L^{-1}T^{-1}$ ). Substitution of (2.57) into (2.54) yields,

$$\begin{aligned} \frac{\partial f(y, t)}{\partial t} &= \frac{Y R(y, t)}{\rho} - b f(y, t) - \frac{f(y, t) Y R(y, t)}{(1 - \epsilon_l) \rho} \\ &\quad - u(y, t) \frac{\partial f(y, t)}{\partial y}. \end{aligned} \quad (2.61)$$

At  $y = 0$ , (2.61) reduces to

$$\frac{\partial f(0, t)}{\partial t} = \frac{Y R(0, t)}{\rho} - b f(0, t) - \frac{f(0, t) Y R(0, t)}{(1 - \epsilon_l) \rho} \quad (2.62)$$

because  $u(y, t) = 0$  at the substratum. The equations (2.58) and (2.61) and the boundary conditions (2.60) (which uses  $u(0, t) = 0$ ) and (2.62) are the transport equations for BAM.

### One-dimensional BAM

#### Diffusional Equations

$$\frac{\partial S(y, t)}{\partial t} = \left( -R(y, t) + \frac{\partial}{\partial y} \left( d \frac{\partial S(y, t)}{\partial y} \right) \right) \quad (2.63)$$

$$\begin{aligned} \frac{dS_b(t)}{dt} = & \frac{1}{V_L} \left( Q \left( S_0 - S_b(t) \right) - \right. \\ & \left. \sigma \left( \frac{D}{L_l} - u(L(t), t) \right) \left( S_b(t) - S(L(t), t) \right) \right) \end{aligned} \quad (2.64)$$

Boundary conditions

$$\frac{\partial S}{\partial y}(0, t) = 0 \quad (2.65)$$

$$\frac{\partial S}{\partial y}(L(t), t) = \frac{D}{L_l} \left( S_b(t) - S(L(t), t) \right) \quad (2.66)$$

#### Transport Equations

$$u(y, t) = \frac{1}{(1 - \epsilon_l)} \int_0^y \frac{Y R(\xi, t)}{\rho} d\xi \quad (2.67)$$

$$\begin{aligned} \frac{\partial f(y, t)}{\partial t} = & \frac{Y R(y, t)}{\rho} - b f(y, t) - \frac{f(y, t) Y R(y, t)}{(1 - \epsilon_l) \rho} \\ & - u(y, t) \frac{\partial f(y, t)}{\partial y} \end{aligned} \quad (2.68)$$

Boundary conditions

$$u_L(t) \equiv u(L(t), t) = \frac{1}{(1 - \epsilon_l)} \int_0^{L(t)} \frac{Y R(\xi, t)}{\rho} d\xi + \delta(t) \quad (2.69)$$

$$u(0, t) = 0 \quad (2.70)$$

$$\frac{\partial f(0, t)}{\partial t} = \frac{Y R(0, t)}{\rho} - b f(0, t) - \frac{f(0, t) Y R(0, t)}{(1 - \epsilon_l) \rho} \quad (2.71)$$

### Zero-dimensional Model

The derivation of the zero-dimensional model equations is based on the approach described in Rittman's model. The four dependent variables and their fundamental units are given in Table 5.

Variables	Physical quantity	Units
$L(t)$	biofilm thickness	$L$
$S_b(t)$	bulk substrate concentration	$M_s L^{-3}$
$S(t)$	average substrate concentration in the biofilm	$M_s L^{-3}$
$f(t)$	average volume fraction of active biomass	dimensionless

Table 5: Unknown dependent variables and their fundamental units in BAM zero-dimensional model

The velocity of the film-water interface comes from (2.60),

$$u_L(t) = \frac{1}{(1 - \epsilon_i)} \frac{Y R(t) L(t)}{\rho} + \delta(t). \quad (2.72)$$

The mass balance for the active biomass in the biofilm is modeled by,

$$\frac{d}{dt}(\sigma L(t)\rho f(t)) = \text{Average growth rate} - \text{inactivation rate} + \text{detachment rate}$$

which is

$$\frac{d}{dt} \left( \sigma L(t)\rho f(t) \right) = Y R(t) L(t) - b\sigma L(t)\rho f(t) + \delta(t)\sigma\rho f(t).$$

Dividing by  $\sigma\rho$  gives

$$\frac{d}{dt} \left( L(t)f(t) \right) = \frac{Y R(t) L(t)}{\rho} - bL(t)f(t) + \delta(t)f(t) \quad (2.73)$$

where  $\delta(t)$  is the detachment rate and  $R(t)$  is the average growth rate of active biomass (average value of  $R(y, t)$  for  $y \in [0, L(t)]$ ). The increase in the concentration of the substrate in the biofilm depends on the rate with which the substrate diffuses into the

biofilm and the rate the substrate is consumed by the active bacteria in the biofilm. The model equation governing the mass balance of the substrate in the biofilm is (see(2.45))

$$\frac{d}{dt} \left( L(t)S(t) \right) = \frac{D}{L_l} \left( S_b(t) - S(t) \right) - R(t)L(t), \quad (2.74)$$

where the first term on right-hand side is due to diffusion of the substrate in the biofilm and  $R(t)$  may be given by Monod kinetics. Assume that the film-water interface is moving with a velocity  $u_L$  perpendicular to the interface. The mass of the substrate in the laminar diffusional sublayer at any time,  $t$ , is  $\sigma L_l(S_b(t) - S(t))$ . The mass balance of the substrate will be given by,

$$\begin{aligned} V_L \frac{dS_b(t)}{dt} &= Q \left( S_0 - S_b(t) \right) - \frac{\sigma D}{L_l} \left( S_b(t) - S(t) \right) \\ &\quad + \sigma u_L(t) \left( S_b(t) - S(t) \right), \end{aligned}$$

which reduces to (see(2.49)),

$$\begin{aligned} \frac{dS_b(t)}{dt} &= \frac{1}{V_L} \left( Q \left( S_0 - S_b(t) \right) - \sigma \left( \frac{D}{L_l} - u_L(t) \right) \right. \\ &\quad \left. \left( S_b(t) - S(t) \right) \right). \end{aligned} \quad (2.75)$$

### Zero-dimensional BAM

$$u_L(t) = \frac{1}{(1 - \epsilon_l)} \frac{Y R(t) L(t)}{\rho} + \delta(t) \quad (2.76)$$

$$\frac{d}{dt} \left( L(t)f(t) \right) = \frac{Y R(t)L(t)}{\rho} - bL(t)f(t) + \delta(t)f(t) \quad (2.77)$$

$$\frac{d}{dt} \left( L(t)S(t) \right) = \frac{D}{L_l} \left( S_b(t) - S(t) \right) - R(t)L(t) \quad (2.78)$$

$$\begin{aligned} \frac{dS_b(t)}{dt} &= \frac{1}{V_L} \left( Q \left( S_0 - S_b(t) \right) - \sigma \left( \frac{D}{L_l} - u_L(t) \right) \right. \\ &\quad \left. \left( S_b(t) - S(t) \right) \right) \end{aligned} \quad (2.79)$$

## Biofilm Growth Model

### One-dimensional Model

Like BAM and Rittman's model, the model developed here is also based on conservation principles. BAM and Rittman's model assume that the volume of the biofilm is negligible compared to the volume of the bulk liquid and hence they treat the volume of the bulk liquid as a constant. If the biofilm grows on the inner surface of a capillary tube or the pore channels of a porous media then the volume of the biofilm and the volume of the bulk liquid will have the same order of magnitude. In this case the volume of the bulk liquid cannot be assumed constant. In the Biofilm Growth Model (BGM), a new set of model equations have been derived which assumes that the volume of the bulk liquid is a function of time. It is assumed that

- The biomass is homogeneous and it may be treated as a continuum.
- The growth of the biofilm is perpendicular to the surface of the film-water interface.
- There is a laminar diffusional sublayer of constant thickness in the bulk liquid.
- The biofilm is made of active and inactive cells of the bacteria and water.

Consider a rectangular box of thickness  $2\Delta y$ , called a control volume, centered at point  $y$  inside the biofilm as shown in Figure 5. If we assume that the box is fixed then, in the box, the volume fraction of the active and inactive biomass and the concentration of the substrate changes with time. The mathematical equations governing the change in the volume fraction of the active and inactive biomass and the substrate concentration are derived from the mass balance equations. The unknown dependent variables determined in this model are shown in Table 6 and the other variables and the parameters used to develop this model are given in Table 7.

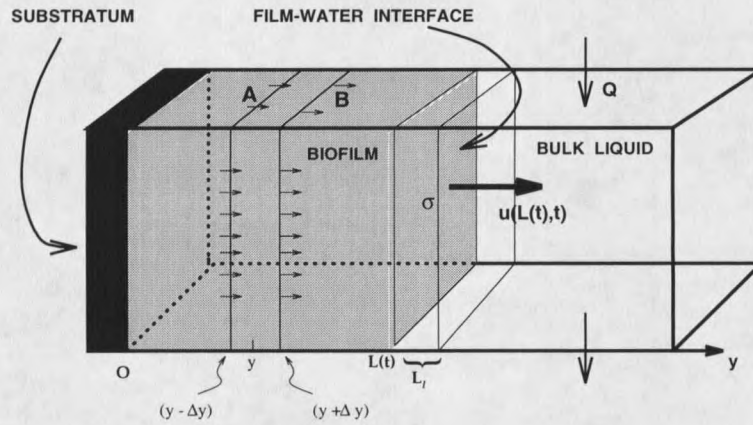


Figure 5: Biofilm on a surface

Variables	Physical quantity	Units
$L(t)$	biofilm thickness	$L$
$V_L(t)$	volume of the bulk liquid	$L^3$
$S_b(t)$	bulk substrate concentration	$M_s L^{-3}$
$S(y, t)$	substrate concentration in the biofilm	$M_s L^{-3}$
$f(y, t)$	volume fraction of active biomass in the biofilm	dimensionless

Table 6: Unknown dependent variables and their fundamental units in the Biofilm Growth Model

Parameters	Physical quantity	Units
$S_0$	substrate concentration in the influent fluid	$M_s L^{-3}$
$\sigma$	area of the film-water interface	$L^2$
$D$	diffusivity coefficient of the substrate through the laminar diffusional sublayer	$L^2 T^{-1}$
$L_l$	thickness of laminar diffusional sublayer	$L$
$d$	diffusivity coefficient of the substrate inside the biofilm	$L^2 T^{-1}$
$V_r$	maximum specific growth rate	$M_s M_x^{-1} T^{-1}$
$K$	Monod constant	$M_s L^{-3}$
$\rho$	biomass density	$M_x L^{-3}$
$b$	inactivation coefficient	$T^{-1}$
$Y$	yield coefficient	$M_x M_s^{-1}$
$\lambda$	detachment coefficient	$L^{-1} T^{-1}$
Variables	Physical quantity	Units
$Q(t)$	volumetric flow rate of the bulk liquid	$L^3 T^{-1}$
$m_f(t)$	mass of the active biofilm at time $t$	$M_x$
$m_s(t)$	mass of the substrate in the film at time $t$	$M_s$
$2\Delta y$	thickness of the rectangular control volume	$L$
$\delta(t)$	detachment rate of the biofilm	$LT^{-1}$
$u(y, t)$	velocity of the biomass particle at $(y, t)$	$LT^{-1}$
$u_L(t)$	velocity of the film-water interface	$LT^{-1}$
$\bar{f}(y, t)$	volume fraction of inactive biomass in the biofilm	dimensionless
$m_{\bar{f}}(t)$	mass of the inactive biofilm at time $t$	$M_x$

Table 7: Parameters and the variables used in Biofilm Growth Model and their fundamental units

**Mass Balance of the Active Biomass** Let  $m_f(t)$  be the mass ( $M_x$ ) of the biofilm inside the box at any time,  $t$ . Then

$$m_f(t) = \sigma \cdot 2\Delta y \cdot \rho \cdot f(y, t) \quad (2.80)$$

where  $\sigma$  is the area ( $L^2$ ) of side  $A$  or side  $B$  of the box,  $2\Delta y$  is the thickness ( $L$ ) of the rectangular control volume,  $\rho$  is the constant density of the biomass ( $M_x L^{-3}$ ), and  $f(y, t)$  is the dimensionless volume fraction of the active biomass.

As the biofilm grows in the box, the biomass enters the box through side  $A$  and leaves the box through side  $B$ . Also the active biomass growth in the biofilm is caused by the substrate consumption and the cell division. We further assume that a certain fraction of the active biomass becomes inactive and it never consumes substrate. The time rate of change of the biomass in the box is

$$\begin{aligned} \frac{\partial m_f(t)}{\partial t} &= \text{influx rate of the biomass through side A} \\ &\quad - \text{outflux rate of the biomass through side B} \\ &\quad + \text{growth rate of the active biomass} \\ &\quad - \text{inactivation rate of the active biomass} \\ &= I_r - O_r + G_r - D_r. \end{aligned} \quad (2.81)$$

Now we will write the mathematical expression for each term in the right-hand side of (2.81) separately.

The influx rate of the biomass through side  $A$ ,  $I_r$  ( $M_x T^{-1}$ ) is given by

$$\begin{aligned} I_r &= \sigma u(y - \Delta y, t) \rho f(y - \Delta y, t) \\ &= \sigma \rho \left( u(y, t) - u_y(y, t)\Delta y + u_{yy}(\eta_1, t) \frac{(\Delta y)^2}{2} \right) \\ &\quad \left( f(y, t) - f_y(y, t)\Delta y + f_{yy}(\zeta_1, t) \frac{(\Delta y)^2}{2} \right) \end{aligned}$$

where  $\eta_1$  and  $\zeta_1$  are points between  $y - \Delta y$  and  $y$ . Ignoring the higher order terms in  $\Delta y$ , the above equation simplifies to

$$I_r = \sigma \rho \left( u(y, t) f(y, t) - u(y, t) f_y(y, t) \Delta y - u_y(y, t) f(y, t) \Delta y \right). \quad (2.82)$$

The outflux rate of the biomass through side B,  $O_r$  ( $M_x T^{-1}$ ) is given by

$$\begin{aligned} O_r &= \sigma u(y + \Delta y, t) \rho f(y + \Delta y, t) \\ &= \sigma \rho \left( u(y, t) + u_y(y, t) \Delta y + u_{yy}(\eta_2, t) \frac{(\Delta y)^2}{2} \right) \\ &\quad \left( f(y, t) + f_y(y, t) \Delta y + f_{yy}(\zeta_2, t) \frac{(\Delta y)^2}{2} \right) \end{aligned}$$

where  $\eta_2$  and  $\zeta_2$  are points between  $y$  and  $y + \Delta y$ . Ignoring the higher order terms in  $\Delta y$ , the above equation simplifies to

$$O_r = \sigma \rho \left( u(y, t) f(y, t) + u(y, t) f_y(y, t) \Delta y + u_y(y, t) f(y, t) \Delta y \right). \quad (2.83)$$

If we assume that the growth of the active biomass is governed by Monod kinetics then  $G_r$  ( $M_x T^{-1}$ ), will be given by,

$$G_r = \frac{Y V_r S(y, t)}{K + S(y, t)} 2 \Delta y \sigma \rho f(y, t), \quad (2.84)$$

where  $Y$  is the yield coefficient ( $M_x M_s^{-1}$ ),  $V_r$  is the maximum growth rate ( $M_s M_x^{-1} T^{-1}$ ), and  $K$  is the Monod constant ( $M_s L^{-3}$ ). Assuming that the inactivation rate of the active biomass is proportional to the mass of the active cells in the box  $D_r$  ( $M_x T^{-1}$ ), will be given by

$$D_r = b 2 \Delta y \sigma \rho f(y, t). \quad (2.85)$$

Using (2.80), (2.82), (2.83), (2.84), and (2.85), (2.81) simplifies to,

$$\begin{aligned} \frac{\partial f(y, t)}{\partial t} &= -u(y, t) f_y(y, t) - u_y(y, t) f(y, t) \\ &\quad + \frac{Y V_r S(y, t) f(y, t)}{K + S(y, t)} - b f(y, t) \end{aligned} \quad (2.86)$$

We have also assumed here that  $\rho$  and  $\sigma$  are constants.

**Mass Balance of the Inactive Biomass** If  $\bar{f}(y, t)$  denotes the volume fraction of the inactive biomass at any instant,  $t$ , then the inactive biomass,  $m_{\bar{f}}(t)$  ( $M_x$ ), is given by

$$m_{\bar{f}}(t) = \sigma \cdot 2\Delta y \cdot \rho \cdot \bar{f}(y, t). \quad (2.87)$$

Also,

$$\begin{aligned} \frac{\partial m_{\bar{f}}(t)}{\partial t} &= \text{influx rate of the inactive biomass through side A} \\ &\quad - \text{outflux rate of the inactive biomass through side B} \\ &\quad + \text{inactivation rate of the active biomass} \\ &= \bar{I}_r - \bar{O}_r + D_r. \end{aligned} \quad (2.88)$$

The influx rate of the inactive biomass through side A,  $\bar{I}_r$  ( $M_x T^{-1}$ ), is given by,

$$\begin{aligned} \bar{I}_r &= \sigma u(y - \Delta y, t) \rho \bar{f}(y - \Delta y, t) \\ &= \sigma \rho \left( u(y, t) - u_y(y, t)\Delta y + u_{yy}(\eta_3, t) \frac{(\Delta y)^2}{2} \right) \\ &\quad \left( \bar{f}(y, t) - \bar{f}_y(y, t)\Delta y + \bar{f}_{yy}(\zeta_3, t) \frac{(\Delta y)^2}{2} \right) \end{aligned}$$

where  $\eta_3$  and  $\zeta_3$  are numbers between  $y - \Delta y$  and  $y$ . Ignoring the higher order terms in  $\Delta y$ , the above equation simplifies to

$$\bar{I}_r = \sigma \rho \left( u(y, t) \bar{f}(y, t) - u(y, t) \bar{f}_y(y, t) \Delta y - u_y(y, t) \bar{f}(y, t) \Delta y \right). \quad (2.89)$$

The outflux rate of the inactive biomass through side B,  $\bar{O}_r$  ( $M_x T^{-1}$ ), is given by

$$\begin{aligned} \bar{O}_r &= \sigma u(y + \Delta y, t) \rho \bar{f}(y + \Delta y, t) \\ &= \sigma \rho \left( u(y, t) + u_y(y, t)\Delta y + u_{yy}(\eta_4, t) \frac{(\Delta y)^2}{2} \right) \\ &\quad \left( \bar{f}(y, t) + \bar{f}_y(y, t)\Delta y + \bar{f}_{yy}(\zeta_4, t) \frac{(\Delta y)^2}{2} \right) \end{aligned}$$

where  $\eta_4$  and  $\zeta_4$  are points between  $y$  and  $y + \Delta y$ . Ignoring the higher order terms in  $\Delta y$ , the above equation simplifies to

$$\bar{O}_r = \sigma \rho \left( u(y, t) \bar{f}(y, t) + u(y, t) \bar{f}_y(y, t) \Delta y + u_y(y, t) \bar{f}(y, t) \Delta y \right). \quad (2.90)$$

Using (2.87), (2.89), (2.90), and (2.85), (2.88) simplifies to,

$$\frac{\partial \bar{f}(y, t)}{\partial t} = -u(y, t) \bar{f}_y(y, t) - u_y(y, t) \bar{f}(y, t) + bf(y, t). \quad (2.91)$$

Adding (2.86) and (2.91) and using the assumption  $f(y, t) + \bar{f}(y, t) = 1 - \epsilon_l$ , we get

$$-(1 - \epsilon_l) u_y(y, t) + \frac{YV_r S(y, t) f(y, t)}{K + S(y, t)} = 0$$

which gives

$$u_y(y, t) = \frac{1}{(1 - \epsilon_l)} \frac{YV_r S(y, t) f(y, t)}{K + S(y, t)}. \quad (2.92)$$

Integrating both sides and using  $u(0, t) = 0$ , we get,

$$u(y, t) = \frac{1}{(1 - \epsilon_l)} \int_0^y \frac{YV_r S(\xi, t) f(\xi, t)}{K + S(\xi, t)} d\xi. \quad (2.93)$$

If we assume that the rate with which the biofilm detaches into the bulk liquid is  $\delta(t)$ , ( $LT^{-1}$ ), then the velocity of the interface will be given by,

$$u_L(t) \equiv u(L(t), t) = \frac{1}{(1 - \epsilon_l)} \int_0^{L(t)} \frac{YV_r S(\xi, t) f(\xi, t)}{K + S(\xi, t)} d\xi + \delta(t). \quad (2.94)$$

The detachment rate,  $\delta(t)$ , is given by  $\delta(t) = -\lambda L^2(t)$ , [25]. The constant  $\lambda$  is called the coefficient of detachment ( $L^{-1}T^{-1}$ ). Using (2.92), (2.86) becomes

$$\begin{aligned} \frac{\partial f(y, t)}{\partial t} &= -u(y, t) f_y(y, t) - \frac{1}{(1 - \epsilon_l)} \frac{YV_r S(y, t) f^2(y, t)}{K + S(y, t)} \\ &\quad + \frac{YV_r S(y, t) f(y, t)}{K + S(y, t)} - bf(y, t) \\ &= -u(y, t) f_y(y, t) + \frac{YV_r S(y, t) f(y, t)}{K + S(y, t)} \left( 1 - \frac{f(y, t)}{1 - \epsilon_l} \right) \\ &\quad - bf(y, t) \\ &= -u(y, t) f_y(y, t) + \frac{YV_r S(y, t) f(y, t) \bar{f}(y, t)}{(K + S(y, t))(1 - \epsilon_l)} - bf(y, t). \end{aligned} \quad (2.95)$$

Similarly using (2.92), (2.91) becomes

$$\frac{\partial \bar{f}(y, t)}{\partial t} = -u(y, t) \bar{f}_y(y, t) - \frac{Y V_r S(y, t) f(y, t) \bar{f}(y, t)}{(K + S(y, t))(1 - \epsilon_l)} + b f(y, t). \quad (2.96)$$

**Mass Balance of the Substrate in the Biofilm** If we denote the substrate concentration in the film by  $S(y, t)$  then the mass of the substrate in the box,  $m_S(t)$ , ( $M_s$ ), will be given by,

$$m_S(t) = \sigma 2\Delta y S(y, t). \quad (2.97)$$

Also,

$$\begin{aligned} \frac{\partial m_S(t)}{\partial t} &= \text{influx rate of the substrate through side A} \\ &\quad - \text{outflux rate of the substrate through side B} \\ &\quad - \text{consumption rate of the substrate} \\ &\quad + \text{diffusion rate of the substrate into the box.} \\ &= \sigma u(y - \Delta y, t) S(y - \Delta y, t) \\ &\quad - \sigma u(y + \Delta y, t) S(y + \Delta y, t) \\ &\quad - \frac{V_r S(y, t)}{K + S(y, t)} (\sigma 2\Delta y) \rho f(y, t) \\ &\quad + d \frac{\partial^2 S(y, t)}{\partial y^2} (\sigma 2\Delta y) \end{aligned} \quad (2.98)$$

where  $d$  is the diffusivity coefficient of the substrate into the biofilm ( $L^2 T^{-1}$ ). Ignoring the higher order terms (2.98) reduces to,

$$\begin{aligned} \frac{\partial m_S(t)}{\partial t} &= \sigma (u(y, t) - u_y(y, t) \Delta y) (S(y, t) - S_y(y, t) \Delta y) \\ &\quad - \sigma (u(y, t) + u_y(y, t) \Delta y) (S(y, t) + S_y(y, t) \Delta y) \\ &\quad - \frac{V_r S(y, t)}{K + S(y, t)} (\sigma 2\Delta y) \rho f(y, t) + d \frac{\partial^2 S(y, t)}{\partial y^2} (\sigma 2\Delta y) \\ &= -(\sigma 2\Delta y) (u(y, t) S_y(y, t) + u_y(y, t) S(y, t)) \\ &\quad - \frac{V_r S(y, t)}{K + S(y, t)} (\sigma 2\Delta y) \rho f(y, t) + d \frac{\partial^2 S(y, t)}{\partial y^2} (\sigma 2\Delta y). \end{aligned} \quad (2.99)$$

Using (2.97), (2.99) reduces to

$$\begin{aligned} \frac{\partial S(y,t)}{\partial t} = & -u(y,t)S_y(y,t) - u_y(y,t)S(y,t) \\ & - \frac{V_r S(y,t)}{K + S(y,t)} \rho f(y,t) + d \frac{\partial^2 S(y,t)}{\partial y^2}. \end{aligned} \quad (2.100)$$

Using (2.92), (2.100) becomes

$$\begin{aligned} \frac{\partial S(y,t)}{\partial t} = & -u(y,t) \frac{\partial S(y,t)}{\partial y} \\ & - \frac{V_r S(y,t) f(y,t)}{K + S(y,t)} \left( \frac{YS(y,t)}{1 - \epsilon_i} + \rho \right) + d \frac{\partial^2 S(y,t)}{\partial y^2}. \end{aligned} \quad (2.101)$$

**Change in the Bulk Liquid Volume** Let us denote the volume of the bulk liquid by  $V_L(t)$  ( $L^3$ ). Then at time  $t + \Delta t$  the volume of the bulk liquid will be given by,

$$V_L(t + \Delta t) = V_L(t) - \sigma u_L(t) \Delta t.$$

As  $\Delta t \rightarrow 0$ , this equation reduces to,

$$\frac{dV_L(t)}{dt} = -\sigma u_L(t). \quad (2.102)$$

**Substrate Concentration in the Bulk Liquid** Let  $S_b(t)$  be the concentration of the substrate in the bulk liquid ( $M_s L^{-3}$ ),  $S_0$  be the concentration of the substrate in the influent fluid ( $M_s L^{-3}$ ), and  $Q(t)$  be the volumetric flow rate of the influent fluid ( $L^3 T^{-1}$ ). Then the rate of change of the total mass of the substrate in the bulk liquid is

$$\begin{aligned} \frac{d}{dt} \left( S_b(t) V_L(t) \right) = & \text{rate of mass increase due to influent fluid} \\ & - \text{rate of mass loss due to fluid flowing out} \\ & - \text{rate of mass loss due to biofilm growth} \end{aligned}$$

—rate of mass loss due to substrate  
diffusion into the film

$$= Q(t)S_0 - Q(t)S_b(t) - u_L(t)\sigma S_b(t) - \frac{\sigma D}{L_l} \left( S_b(t) - S(L(t), t) \right) \quad (2.103)$$

which gives,

$$S_b(t) \frac{dV_L(t)}{dt} + V_L(t) \frac{dS_b(t)}{dt} = Q(t)S_0 - Q(t)S_b(t) - u_L(t)\sigma S_b(t) - \frac{\sigma D}{L_l} \left( S_b(t) - S(L(t), t) \right). \quad (2.104)$$

Using (2.102) this simplifies to,

$$\frac{dS_b(t)}{dt} = \frac{1}{V_L(t)} \left( Q(t)(S_0 - S_b(t)) - \frac{\sigma D}{L_l} (S_b(t) - S(L(t), t)) \right). \quad (2.105)$$

### One-dimensional BGM

$$\frac{\partial f(y, t)}{\partial t} = -u(y, t)f_y(y, t) + \frac{YV_r S(y, t)f(y, t)\bar{f}(y, t)}{(K + S(y, t))(1 - \epsilon_l)} - bf(y, t) \quad (2.106)$$

$$\frac{\partial S(y, t)}{\partial t} = -u(y, t) \frac{\partial S(y, t)}{\partial y} - \frac{V_r S(y, t)f(y, t)}{K + S(y, t)} \left( \frac{YS(y, t)}{1 - \epsilon_l} + \rho \right) + d \frac{\partial^2 S(y, t)}{\partial y^2} \quad (2.107)$$

$$\bar{f}(y, t) = 1 - \epsilon_l - f(y, t) \quad (2.108)$$

$$u(y, t) = \frac{1}{(1 - \epsilon_l)} \int_0^y \frac{YV_r S(\xi, t)f(\xi, t)}{K + S(\xi, t)} d\xi \quad (2.109)$$

$$\frac{dV_L(t)}{dt} = -\sigma u_L(t) \quad (2.110)$$

$$\frac{dS_b(t)}{dt} = \frac{1}{V_L(t)} \left( Q(t)(S_0 - S_b(t)) - \frac{\sigma D}{L_l} (S_b(t) - S(L(t), t)) \right) \quad (2.111)$$

Boundary conditions

$$\frac{\partial S}{\partial y}(0, t) = 0 \quad (2.112)$$

$$d \frac{\partial S}{\partial y}(L(t), t) = \frac{D}{L_i} \left( S_b(t) - S(L(t), t) \right) \quad (2.113)$$

$$u(0, t) = 0 \quad (2.114)$$

$$u_L(t) \equiv u(L(t), t) = \frac{1}{(1 - \epsilon_i)} \int_0^{L(t)} \frac{YV_r S(\xi, t) f(\xi, t)}{K + S(\xi, t)} d\xi + \delta(t) \quad (2.115)$$

and

$$\frac{\partial f}{\partial t}(0, t) = \frac{YV_r S(0, t) f(0, t) \bar{f}(0, t)}{(K + S(0, t))(1 - \epsilon_i)} - bf(0, t). \quad (2.116)$$

### Zero-dimensional Model

The derivation of zero-dimensional BGM is also based on the idea described in Rittman's model. The unknown dependent variables determined by this model are given in Table 8. The rate of change of the active biomass depends on the growth

Variables	Physical quantity	Units
$L(t)$	biofilm thickness	$L$
$V_L(t)$	volume of the bulk liquid	$L^3$
$S_b(t)$	bulk substrate concentration	$M_s L^{-3}$
$S(t)$	average substrate concentration in the biofilm	$M_s L^{-3}$
$f(t)$	average volume fraction of active biomass in the biofilm	dimensionless

Table 8: Unknown dependent variables and their fundamental units in the zero-dimensional Biofilm Growth Model

rate of active biomass, inactivation rate of active biomass and the detachment rate.

A mathematical expression for the rate of change of active biomass may be given by

(see (2.95))

$$\frac{d}{dt} \left( \sigma \rho f(t) L(t) \right) = \left( \frac{YV_r S(t)}{(K + S(t))} - b \right) \sigma \rho L(t) f(t) + \delta(t) \sigma \rho f(t).$$

Using the chain rule and the assumption that  $\rho$  and  $\sigma$  are constants, the above equation reduces to

$$\frac{df(t)}{dt} = -\frac{f(t)}{L(t)} \frac{dL(t)}{dt} + \left( \frac{YV_r S(t)}{(K + S(t))} - b + \frac{\delta(t)}{L(t)} \right) f(t). \quad (2.117)$$

The inactive biomass increases as the active biomass becomes inactive and it decreases as the biofilm detaches at the interface between the film and the liquid. The rate of change of inactive biomass can be given by,

$$\frac{d}{dt} \left( \sigma \rho \bar{f}(t) L(t) \right) = b \sigma \rho L(t) f(t) + \delta(t) \sigma \rho \bar{f}(t),$$

which simplifies to,

$$\frac{d\bar{f}(t)}{dt} = -\frac{\bar{f}(t)}{L(t)} \frac{dL(t)}{dt} + b f(t) + \frac{\delta(t)}{L(t)} \bar{f}(t).$$

Adding this to (2.117) and using the assumption that  $f(t) + \bar{f}(t) + \epsilon_l = 1$  we get,

$$\frac{dL(t)}{dt} = \frac{1}{1 - \epsilon_l} \frac{Y V_r L(t) S(t) f(t)}{K + S(t)} + \delta(t). \quad (2.118)$$

The average rate of change of the substrate in the biofilm depends on the consumption rate of the substrate and the diffusion rate of the substrate into the film. A mathematical expression for the rate of change of the substrate in the film may be given by,

$$\frac{d}{dt} \left( \sigma S(t) L(t) \right) = \frac{\sigma D}{L_l} \left( S_b(t) - S(t) \right) - \frac{V_r S(t)}{K + S(t)} \rho \sigma L(t) f(t)$$

which reduces to

$$\frac{dS(t)}{dt} = -\frac{S(t)}{L(t)} \frac{dL(t)}{dt} + \frac{D}{L_l L(t)} \left( S_b(t) - S(t) \right) - \frac{V_r S(t) \rho f(t)}{K + S(t)}. \quad (2.119)$$

The substrate concentration in the bulk liquid from (2.105) is

$$\frac{dS_b(t)}{dt} = \frac{1}{V_L(t)} \left( Q(t) (S_0 - S_b(t)) - \frac{\sigma D'}{L_l} (S_b(t) - S(t)) \right) \quad (2.120)$$

and the volume of the bulk liquid from (2.102) is,

$$\frac{dV_L(t)}{dt} = -\sigma \frac{dL(t)}{dt}. \quad (2.121)$$

### Zero-dimensional BGM

$$\frac{df(t)}{dt} = -\frac{f(t)}{L(t)} \frac{dL(t)}{dt} + \left( \frac{Y V_r S(t)}{K + S(t)} - b + \frac{\delta(t)}{L(t)} \right) f(t) \quad (2.122)$$

$$\frac{dL(t)}{dt} = \frac{1}{1 - \epsilon_t} \frac{YV_r L(t) S(t) f(t)}{K + S(t)} + \delta(t) \quad (2.123)$$

$$\frac{dS(t)}{dt} = -\frac{S(t)}{L(t)} \frac{dL(t)}{dt} + \frac{D}{L_i L(t)} \left( S_b(t) - S(t) \right) - \frac{V_r S(t) \rho f(t)}{K + S(t)} \quad (2.124)$$

$$\frac{dS_b(t)}{dt} = \frac{1}{V_L(t)} \left( Q(t)(S_0 - S_b(t)) - \frac{\sigma D}{L_i} (S_b(t) - S(t)) \right) \quad (2.125)$$

$$\frac{dV_L(t)}{dt} = -\sigma \frac{dL(t)}{dt} \quad (2.126)$$

## CHAPTER 3

# Comparison of the Biofilm Models

### Introduction

When the biofilm grows on the pore surface of the porous media, the pore volume decreases which effects the porosity and the permeability of the porous media [2], [5], [9], [18], [23]. The physical properties, porosity and permeability, of the porous media are defined in Chapter 4. Experimentally it has been shown that the change in the porosity and the permeability affects the flow rate of the bulk fluid through the pore channels [5], [18]. How fast do the pore channels clog? How does the biofilm growth affect the flow rate through the porous media? To answer these questions we must have an efficient model which describes the biofilm growth on a surface and can be combined easily with porous media flow models [2], [9], [23]. In this chapter the numerical results of the three models (BGM, BAM, and Rittman's model) developed in Chapter 2 are compared. We seek the most efficient mathematical model which describes the biofilm growth on a surface. The Biofilm Growth Model (BGM) assumes that the volume of the bulk liquid is a function of time rather than a constant. In the next two sections the numerical solutions of one-dimensional and zero-dimensional BGM are discussed and compared. Then the solutions of the zero-dimensional Rittman's model, BAM, and BGM (restricted so that is comparable to BAM and Rittman's model) are discussed in the fourth, fifth, and sixth sections, respectively. The last section provides a comparison of all three zero dimensional models (where again BGM is restricted to be like BAM and Rittman's model).

Both the one-dimensional Rittman's model and the one-dimensional BAM are accepted models for biofilm growth and the zero-dimensional Rittman's model has been compared to the one-dimensional version [12]. This comparison of the three different zero-dimensional models validates the use of the zero-dimensional BGM for the porous media applications considered in this dissertation.

### Solution of One-dimensional BGM

The system of equations (2.106)-(2.116) from the one-dimensional BGM are solved numerically for the dependent variables given in Table 6 and then the results are discussed. The spatial derivatives in (2.106) and (2.107) are replaced by their finite difference approximations

$$\frac{\partial}{\partial y} (f(y, t)) = \frac{f(y + \Delta y, t) - f(y - \Delta y, t)}{2\Delta y}, \quad (3.1)$$

$$\frac{\partial}{\partial y} (S(y, t)) = \frac{S(y + \Delta y, t) - S(y - \Delta y, t)}{2\Delta y}, \quad (3.2)$$

and

$$\frac{\partial^2}{\partial y^2} (S(y, t)) = \frac{S(y + \Delta y, t) - 2S(y, t) + S(y - \Delta y, t)}{(\Delta y)^2}. \quad (3.3)$$

Also the velocity,  $u(y, t)$ , which is an integral given in (2.109), has been approximated using the trapezoidal rule [3], [15] and  $u(y, t)$  has been replaced with its approximation in (2.106), (2.107), and (2.110). The trapezoidal rule is explained briefly below.

**Trapezoidal Rule** Let  $F(y)$  be a continuous function over  $[a, b]$  as shown in Figure 6. Divide  $[a, b]$  into  $n$  equal subintervals of length  $\Delta y = \frac{b-a}{n}$  and define  $y_i = a + i\Delta y$ ,  $i = 0, \dots, n$ . Then the approximation of the integral of  $F(y)$  over the interval  $[y_{i-1}, y_i]$  is given by

$$\int_{y_{i-1}}^{y_i} F(y) dy = \frac{F(y_i) + F(y_{i-1})}{2} \Delta y \quad (3.4)$$

and the integral of  $F(y)$  over the interval  $[a, b]$  is given by

$$\int_a^b F(y)dy = \sum_{i=1}^n \frac{F(y_i) + F(y_{i-1})}{2} \Delta y. \quad (3.5)$$

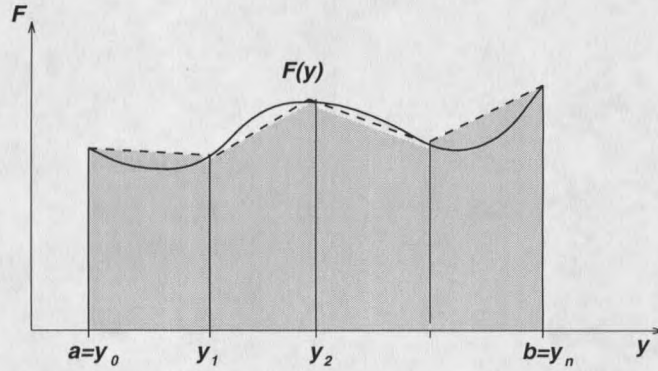


Figure 6: Function  $F(y)$  and the approximation of its integral over  $[a, b]$

After replacing all the spatial derivatives and the velocity,  $u(y, t)$ , in (2.106), (2.107), (2.110), and (2.111) with their approximations, a system of ordinary differential equations results. The system of ordinary differential equations is then solved using the MATLAB (version 4.2a) package 'ODE23s'. The software 'ODE23s' solves systems of stiff ordinary differential equations using the modified Rosenbrock method. A computer code for the subroutine 'ODE23s' is given in Appendix A. More information on 'ODE23s' can be found in [24] and the Rosenbrock method is explained in [13]. The modified Rosenbrock method can be found in [27]. The values of the parameters and the initial values of the dependent variables used to run the simulation are based on [12], [25] and are displayed in Table 9. All codes are developed in MATLAB and run on a DECstation 5000/240. The computer code which approximates the solution of the one-dimensional BGM equations is given in Appendix B.

Parameters	Values	Units
$K$	0.0001	mg/cm <sup>3</sup>
$V_r$	4.3	mg/(mg day)
$Y$	.5	mg/mg
$b$	.35	day <sup>-1</sup>
$D$	1.3	cm <sup>2</sup> /day
$Q(t) \forall t$	1100	cm <sup>3</sup> /day
$\sigma$	1	cm <sup>2</sup>
$L_l$	.8	cm
$\epsilon_l$	.8	dimensionless
$d$	1.04	cm <sup>2</sup> / day
$\rho$	12.2	mg/cm <sup>3</sup>
$S_0$	.02	mg/cm <sup>3</sup>
$\lambda$	500	cm <sup>-1</sup> day <sup>-1</sup>
Variables	Initial Values	Units
$S_b(0)$	.04	mg/cm <sup>3</sup>
$L(0)$	.00005	cm
$S(y, 0) \forall y$	.00004	mg/cm <sup>3</sup>
$f(y, 0) \forall y$	.15	dimensionless
$V_L(0)$	.03	cm <sup>3</sup>

Table 9: Parameter values and initial values for one-dimensional BGM

### Change in the Biofilm Thickness

The biofilm thickness is governed by growth and detachment. The bacteria in the biofilm consume the substrate and multiply. Bacteria near the substratum get less food than the bacteria near the film-water interface, hence the bacteria near the interface grow faster than the bacteria near the substratum. The cumulative growth of each mass particle determines the growth rate of the biofilm thickness,  $L(t)$ . Figure 7 shows that the biofilm thickness initially (for the first .5 days) grows slowly then the growth rate increases and the biofilm thickness grows rapidly over the next 1.5 days. The growth after 2 days is very slow (see Figure 7 and Table 11). The biofilm thickness reaches a steady state at .008202 cm after 4 days.

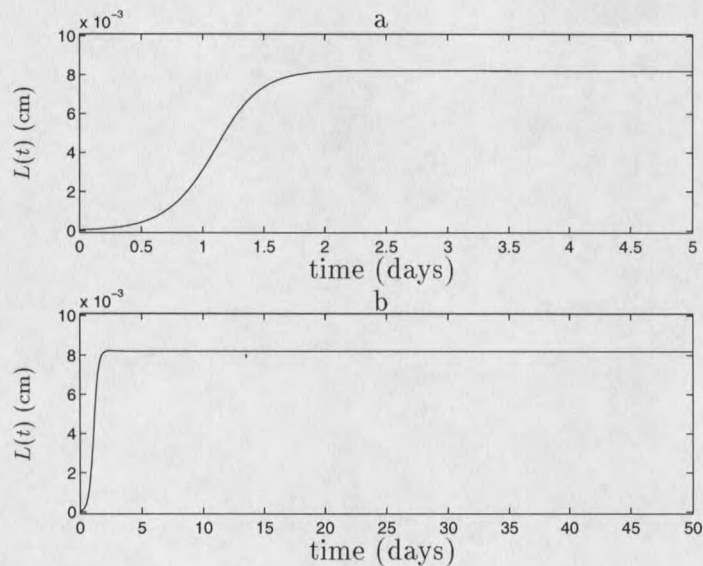


Figure 7: The thickness of the biofilm,  $L(t)$ , over 5 days (a) and 50 days (b) for the one-dimensional BGM

### Change in the Volume of the Bulk Liquid

As the biofilm thickness grows, the volume of the bulk liquid,  $V_L(t)$ , decreases. It is clear from Figures 7 and 8 that when biofilm thickness reaches its steady state, the

volume of the bulk liquid also reaches its steady state. We observe a 27% decrease in the volume over the first 2 days of bacterial growth. The bulk liquid volume then reaches its steady state of  $.02185 \text{ cm}^3$  after 4 days (see Table 12).

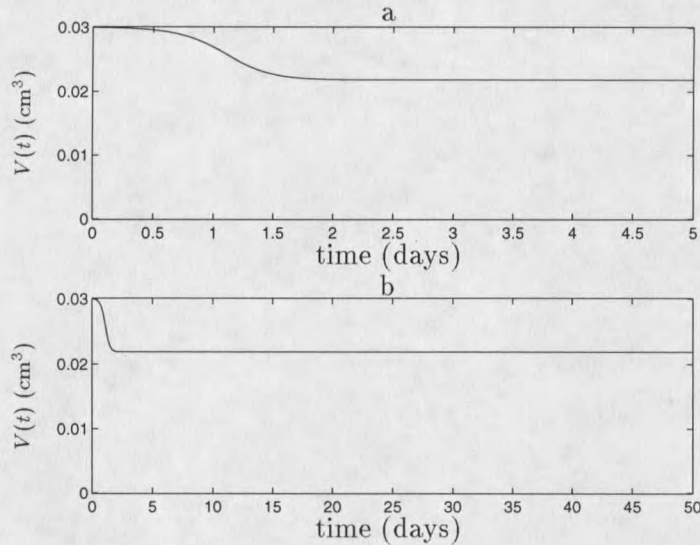


Figure 8: The volume of the bulk liquid,  $V_L(t)$ , over 5 days (a) and 50 days (b) for the one-dimensional BGM

### Change in the Substrate Concentration in the Biofilm

The substrate concentration,  $S(y, t)$ , at a fixed point in the biofilm depends on the distance of the point from the film-water interface. A point near the film-water interface has a much higher substrate concentration than a point near the substratum. This is due to the fact that a significant fraction of the substrate molecules, which diffuse into the biofilm, are consumed by the bacteria before they get close to the substratum. When we fix a point in the biofilm and calculate the substrate concentration at that point, we observe that as biofilm grows, the substrate concentration at that point decreases because as biofilm grows, the distance between the point and the film-water interface increases. The graphs of substrate concentration at two

points  $y_1$  and  $y_2$  are shown in Figures 9 and 10.  $y_1$  is a point which is at 20% of the biofilm thickness,  $L(t)$ , from the substratum and  $y_2$  is a point which is at 80% of the biofilm thickness from the substratum. Thus  $y_1$  and  $y_2$  move as the biofilm thickness increases. Since the biofilm is initially very thin, the substrate from the bulk liquid diffuses very quickly into the film and the substrate concentration rises from its initial value,  $.00004 \text{ mg/cm}^3$ , to  $.04 \text{ mg/cm}^3$ , which is the initial bulk substrate concentration,  $S_b(0)$ . Then the substrate concentration in the biofilm very rapidly decreases to  $.02 \text{ mg/cm}^3$  which is the substrate concentration of the influent fluid (see Figure 9). Figure 9 and Table 13 show that between .5 days and 1.5 days the substrate concentration at  $y_1$  decreases faster than the substrate concentration at  $y_2$ . The substrate concentrations  $S(y_1, t)$  and  $S(y_2, t)$  both attain their steady states after 4 days. The steady state value of  $S(y_2, t)$  is  $.01566 \text{ mg/cm}^3$  which is significantly higher than the steady state value of  $S(y_1, t)$  ( $.000066 \text{ mg/cm}^3$ ) because  $y_2$  is closer to the interface than  $y_1$ .

### Change in the Volume Fraction of the Active and Inactive Bacteria

It has been assumed in this model that a constant fraction,  $\epsilon_l = .8$ , of the biofilm is water. The volume fractions of active and inactive bacteria change between 0 and  $(1 - \epsilon_l) = .2$  and their sum remains a constant,  $(1 - \epsilon_l) = .2$ . In the case of high substrate concentration in the biofilm, the active bacteria multiply faster than they inactivate (die). Hence in any arbitrary volume of the biofilm the relative fraction of the active bacteria,  $f(y, t)$ , increases and the volume fraction of the inactive bacteria,  $\bar{f}(y, t)$ , decreases. The volume fractions of the active bacteria at points  $y_1$  (which is at 20% of the biofilm thickness from the substratum) and  $y_2$  (which is at 80% of the biofilm thickness from the substratum) are displayed in Figure 11 (over 2.5 days) and Figure 12 (over 50 days). Initially, when the biofilm is thin, the volume fraction

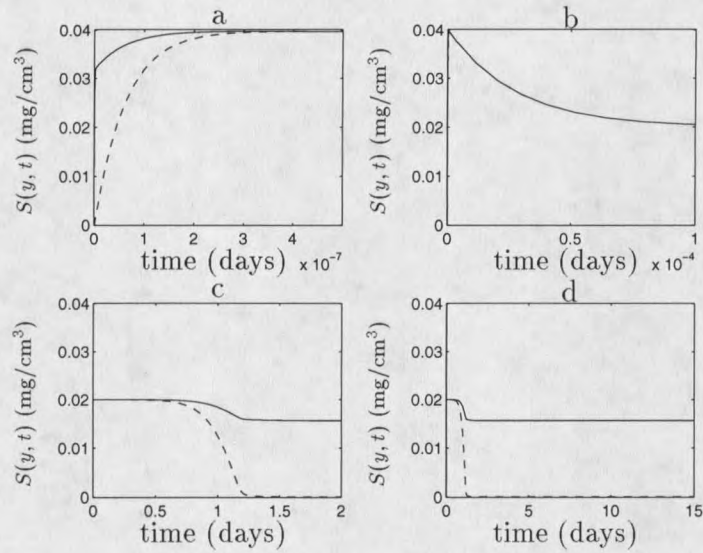


Figure 9: The substrate concentration,  $S(y, t)$ , in the biofilm at points  $y_1$  (dashed line) and  $y_2$  (solid line) in the biofilm over  $10^{-7}$  days (a), .0001 days (b), 2 days (c), and 15 days (d), for the one-dimensional BGM

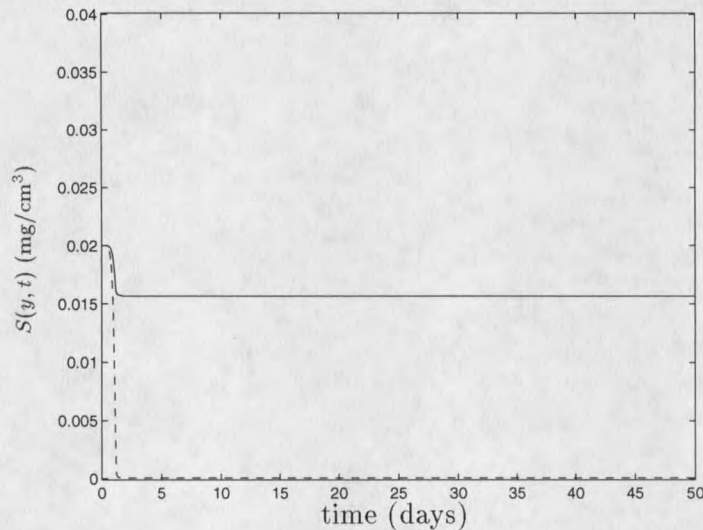


Figure 10: The substrate concentration,  $S(y, t)$ , at points  $y_1$  (dashed line) and  $y_2$  (solid line) in the biofilm over 50 days for the one-dimensional BGM

of the active bacteria at  $y_1$ ,  $f(y_1, t)$ , and the volume fraction of the active bacteria at  $y_2$ ,  $f(y_2, t)$ , increase with almost the same rate. After 1.2 days, when the biofilm thickness is significantly large, the bacteria at  $y_1$  do not get enough substrate hence  $f(y_1, t)$  begins to decrease, however  $f(y_2, t)$  continues to increase. Figure 12 and Table 15 show that  $f(y_1, t)$  and  $f(y_2, t)$ , after 5 days, attain their steady states at .173465 and .189406, respectively.

The volume fraction of inactive biomass,  $\bar{f}(y, t)$ , changes with the change in the volume fraction of active biomass,  $f(y, t)$ , such that at any point  $y^*$  and time  $t^*$  the sum of  $f(y^*, t^*)$  and  $\bar{f}(y^*, t^*)$  remains 0.2. Figure 12 and Table 16 show that  $\bar{f}(y_1, t)$  and  $\bar{f}(y_2, t)$ , after 5 days, attain their steady states at .026534 and .010594, respectively.

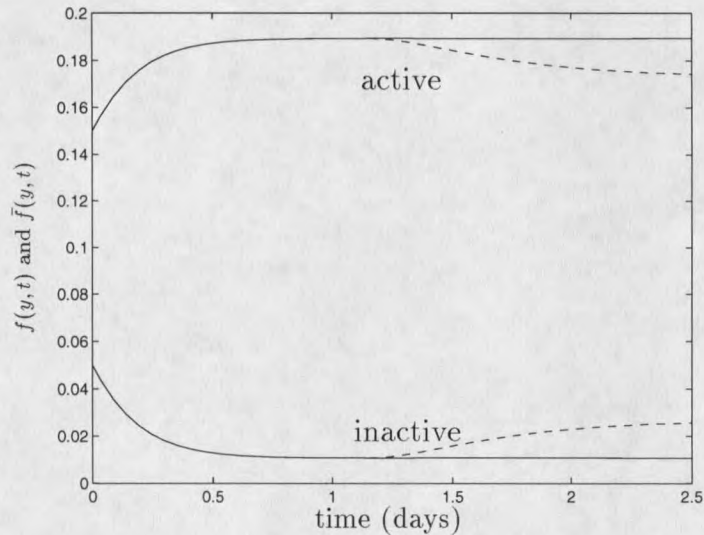


Figure 11: The active biomass volume fraction,  $f(y, t)$ , and the inactive biomass volume fraction,  $\bar{f}(y, t)$ , at points  $y_1$  (dashed line) and  $y_2$  (solid line) over 2.5 days for the one-dimensional BGM

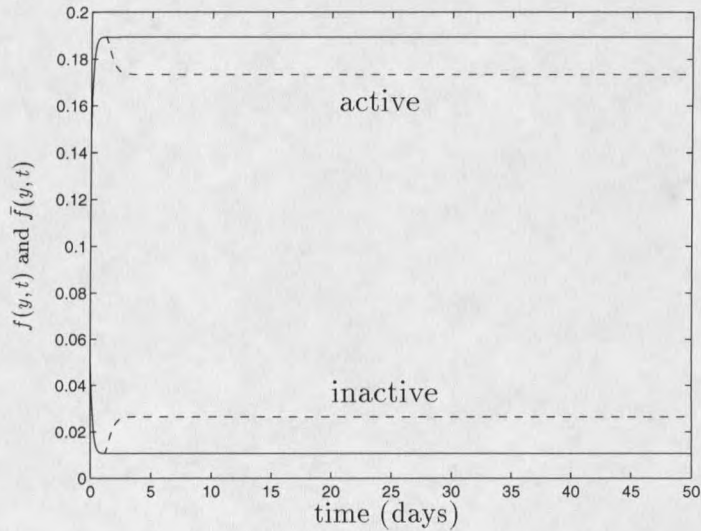


Figure 12: The active biomass volume fraction,  $f(y, t)$ , and the inactive biomass volume fraction,  $\bar{f}(y, t)$ , at points  $y_1$  (dashed line) and  $y_2$  (solid line) over 50 days for the one-dimensional BGM

### Change in the Substrate Concentration in the Bulk Liquid

Figure 13 shows that the substrate concentration,  $S_b(t)$ , in the bulk liquid very rapidly (in .0004 days) approaches its steady state value which is the constant value  $S_0 = .02 \text{ mg/cm}^3$ . This is the concentration of the substrate in the influent fluid. Since the volumetric flow rate is very high, the substrate solution is continuously being replaced with new solution of constant concentration,  $S_0 = .02 \text{ mg/cm}^3$ . This is shown in Figure 13 and the numerical values of  $S_b(t)$  are displayed in Table 17.

### Comparison of Zero- and One-dimensional BGM

The system of equations (2.122) - (2.126) from the zero-dimensional BGM are solved numerically for the dependent variables given in Table 8 and then the results are discussed. The solution is determined using 'ODE23s' from MATLAB (version 4.2a). The computer code which approximates the solution of the zero-dimensional

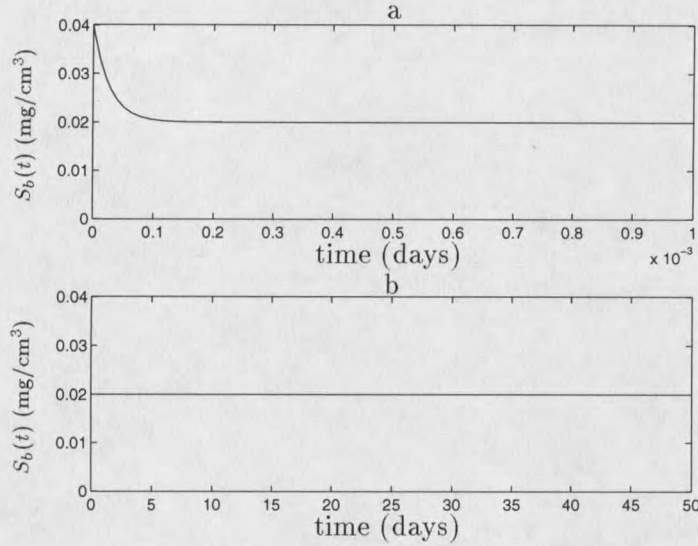


Figure 13: The substrate concentration,  $S_b(t)$ , in the bulk liquid over .001 days (a) and 50 days (b) for the one-dimensional BGM

BGM equations is given in Appendix C.

Replacing  $\frac{dL(t)}{dt}$  in equations (2.122), (2.124) and (2.126) with the right-hand side of (2.123) yields the following system of differential equations:

$$\frac{df(t)}{dt} = \frac{YV_r S(t)f(t)}{K + S(t)} \left( 1 - \frac{f(t)}{1 - \epsilon_l} \right) - bf(t) \quad (3.6)$$

$$\frac{dL(t)}{dt} = \frac{1}{1 - \epsilon_l} \frac{YV_r L(t)S(t)f(t)}{K + S(t)} + \delta(t) \quad (3.7)$$

$$\frac{dS(t)}{dt} = -\frac{V_r S(t)f(t)}{K + S(t)} \left( \rho + \frac{S(t)Y}{1 - \epsilon_l} \right) - \frac{\delta(t)S(t)}{L(t)} + \frac{D}{L_l L(t)} \left( S_b(t) - S(t) \right) \quad (3.8)$$

$$\frac{dS_b(t)}{dt} = \frac{1}{V_L(t)} \left( Q(t)(S_0 - S_b(t)) - \frac{\sigma D}{L_l} (S_b(t) - S(t)) \right) \quad (3.9)$$

$$\frac{dV_L(t)}{dt} = -\sigma \left( \frac{1}{1 - \epsilon_l} \frac{YV_r L(t)S(t)f(t)}{K + S(t)} + \delta(t) \right) \quad (3.10)$$

The model equation for the detachment function,  $\delta(t)$ , that we have used here, is, [25]

$$\delta(t) = -\lambda(L(t))^2 \quad (3.11)$$

where  $\lambda$  ( $L^{-1}T^{-1}$ ) is the detachment coefficient.

This system is solved for five unknown variables; substrate in the bulk fluid,  $S_b(t)$ , thickness of the biofilm,  $L(t)$ , average substrate concentration in the biofilm,  $S(t)$ , average volume fraction of the biomass in the biofilm,  $f(t)$ , and the volume of the bulk liquid,  $V_L(t)$ . The parameter values and the initial values of the variables are given in Table 10 and are the same as those used for the one-dimensional BGM (see Table 9). The numerical approximation of these functions is displayed in Figures 14 through 27 and in Tables 11 through 17. A comparison of the values of the variables from the one-dimensional and zero-dimensional models is also given.

Parameters	Values	Units
$K$	0.0001	mg/cm <sup>3</sup>
$V_r$	4.3	mg/(mg day)
$Y$	.5	mg/mg
$b$	.35	day <sup>-1</sup>
$D$	1.3	cm <sup>2</sup> /day
$Q(t) \forall t$	1100	cm <sup>3</sup> /day
$\sigma$	1	cm <sup>2</sup>
$L_l$	.8	cm
$\epsilon_l$	.8	dimensionless
$\rho$	12.2	mg/cm <sup>3</sup>
$S_0$	.02	mg/cm <sup>3</sup>
$\lambda$	500	cm <sup>-1</sup> day <sup>-1</sup>
Variables	Values	Units
$S_b(0)$	.04	mg/cm <sup>3</sup>
$L(0)$	.00005	cm
$S(0)$	.00004	mg/cm <sup>3</sup>
$f(0)$	.15	dimensionless
$V_L(0)$	.03	cm <sup>3</sup>

Table 10: Parameter values and initial values for the zero-dimensional BGM

### Change in the Biofilm Thickness

Figure 14 shows that the biofilm thickness,  $L(t)$ , increases slowly over the first .5 days and over the next 1.5 days it grows rapidly. The growth rate of the biofilm thickness is very slow after 2.5 days and a steady state is reached after 8 days of .008152 cm. A comparison of  $L(t)$  computed from one-dimensional BGM and zero-dimensional BGM is shown in Figure 15 and the numerical values are displayed in Table 11. The steady state in the zero-dimensional BGM is attained after a longer time at a smaller value than in the one-dimensional BGM but qualitatively both graphs are very similar.

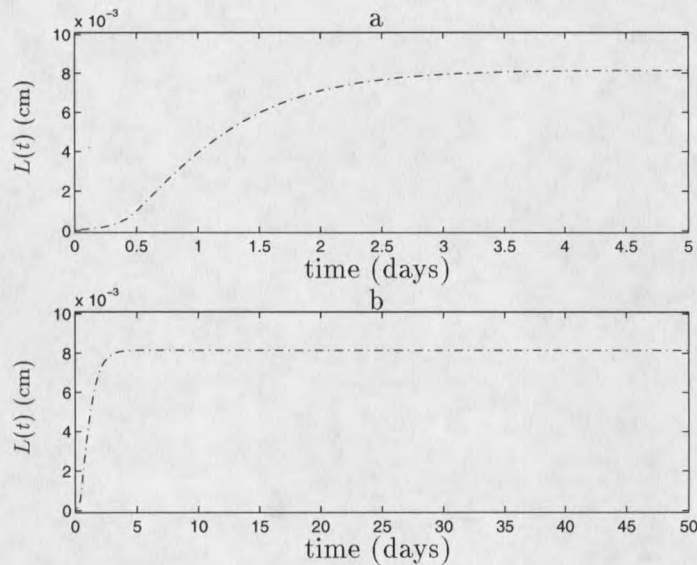


Figure 14: Biofilm thickness,  $L(t)$ , over 5 days (a) and 50 days (b) for the zero-dimensional BGM

### Change in the Volume of the Bulk Liquid

Figure 16 and Table 12 show that initially (over the first .5 days) the volume,  $V_L(t)$ , of the bulk liquid decreases slowly. But over the next 1.5 days,  $V_L(t)$  decreases rapidly because between .5 days and 2 days the biofilm thickness,  $L(t)$ , increases very fast

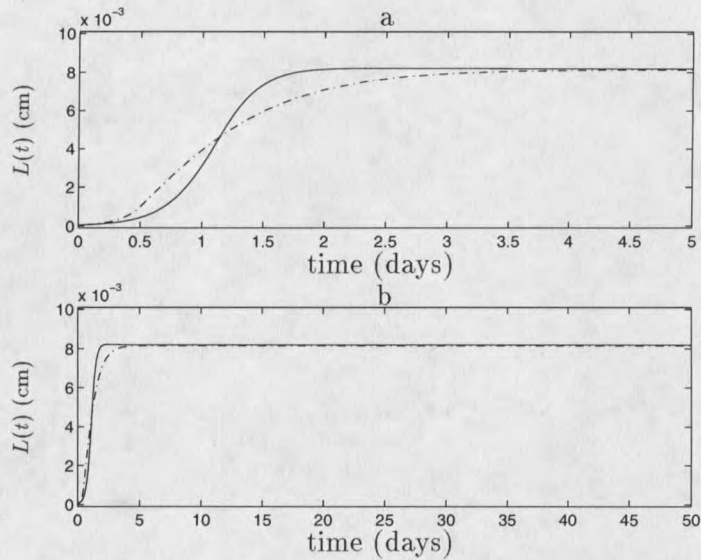


Figure 15: Biofilm thickness,  $L(t)$ , over 5 days (a) and 50 days (b) for the zero-dimensional (dash-dot line) and one-dimensional (solid line) BGM

(leaving less room for the bulk liquid). Notice that  $V_L(t)$  reaches a steady state of  $.021898 \text{ cm}^3$  after 9 days. Table 12 also shows that  $V_L(t)$  in the zero-dimensional model attains its steady state at a slightly higher value than it does in the one-dimensional model because the steady biofilm thickness in the zero-dimensional model is smaller than it is in the one-dimensional model.

### Change in Substrate Concentration in the Biofilm

Initially, because of the high substrate concentration difference across the film-water interface ( $.00004 \text{ mg/cm}^3$  in the biofilm and  $.04 \text{ mg/cm}^3$  in the bulk liquid), the substrate diffuses rapidly from high to low concentration. This causes the substrate concentration,  $S(t)$ , in the biofilm to increase rapidly. Simultaneously the substrate concentration in the bulk liquid,  $S_b(t)$ , decreases rapidly because it is replaced with the influent liquid of constant substrate concentration,  $S_0 = .02 \text{ mg/cm}^3$ . After about  $.00006$  days (or 5.2 seconds)  $S(t)$  increases to  $.0222 \text{ mg/cm}^3$  (see Figure 18) and  $S_b(t)$

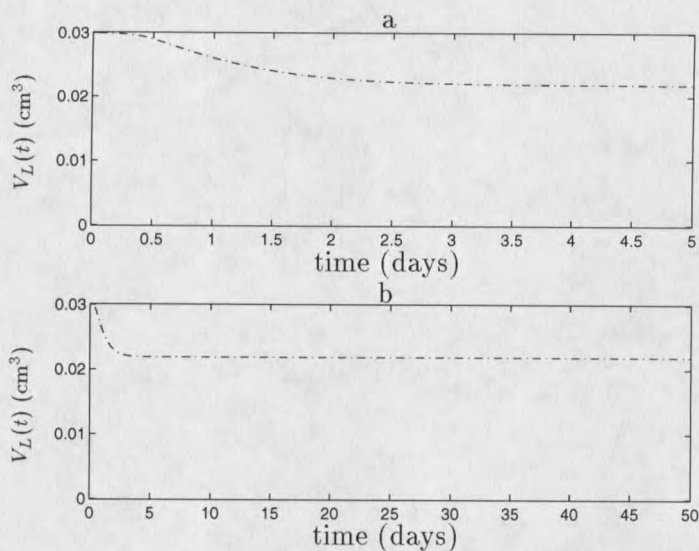


Figure 16: The bulk fluid volume,  $V_L(t)$ , over 5 days (a) and 50 days (b) for the zero-dimensional BGM

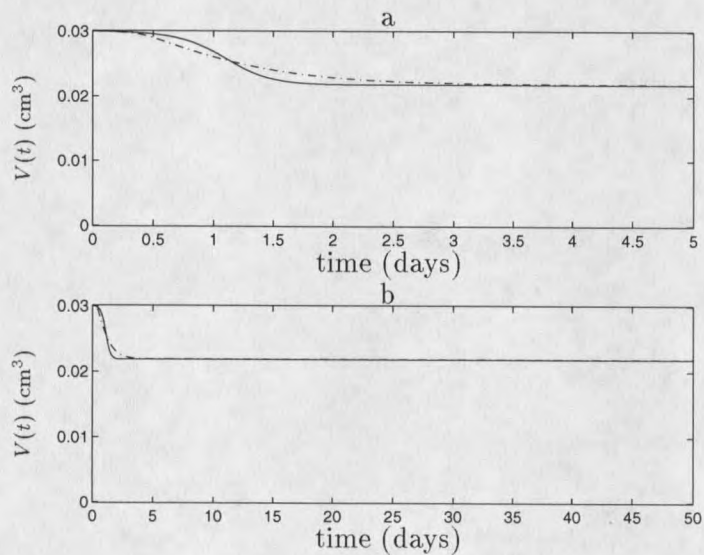


Figure 17: The bulk fluid volume,  $V(t)$ , over 5 (a) days and 50 days (b) for the zero-dimensional (dash-dot line) and one-dimensional (solid line) BGM

decreases to  $.0222 \text{ mg/cm}^3$  (see Figure 27). Since the concentration difference across the film-water interface is zero there (at  $t = .00006$  days),  $S(t)$  stops increasing, which can be visualized in Figure 18 as the slope of  $S(t)$  is zero at  $t = .00006$  days. Figure 27 shows that after  $.00006$  days,  $S_b(t)$  continues to decrease which causes a concentration difference across the film water interface (high in the biofilm and low in the bulk fluid). Therefore the substrate from the biofilm diffuses into the bulk liquid and decreases to a value close to  $S_0 = .02 \text{ mg/cm}^3$ . As biofilm grows, the substrate in the biofilm get consumed faster causing a slow decrease in  $S(t)$  which can be seen in Figure 19. After 1.5 days, when the biofilm thickness becomes significantly large, the substrate consumption rate increases which causes relatively faster decrease in the substrate concentration. A comparison of the substrate concentration,  $S(t)$ , from the zero-dimensional BGM and the substrate concentrations  $S(y_1, t)$  and  $S(y_2, t)$  from one-dimensional BGM is shown in Figure 20 (over 2.5 days) and Figure 22 (over 50 days). The numerical values of  $S(t)$ ,  $S(y_1, t)$ , and  $S(y_2, t)$  are given in Table 13 and Table 14. Figure 22 and Table 14 show that  $S(t)$  reaches its steady state after 4 days at  $.003965 \text{ mg/cm}^3$  which is between the steady state values of  $S(y_1, t)$  ( $.000066 \text{ mg/cm}^3$ ) and  $S(y_2, t)$  ( $.01566 \text{ mg/cm}^3$ ).

### Change in the Volume Fraction of Active and Inactive Bacteria

The graphs of the volume fraction of active biomass,  $f(t)$ , and the volume fraction of inactive biomass,  $\bar{f}(t)$ , are shown in Figure 23 (over 2.5 days) and Figure 24 (over 50 days). The numerical values of  $f(t)$  are displayed in Table 15 and the numerical values of  $\bar{f}(t)$  are displayed in Table 16. The volume fraction of active biomass increases from its initial value  $.15$  to its steady state value  $.1821$  and the volume fraction of the inactive biomass decreases from its initial value  $.05$  to its steady state value  $.0179$ . Also notice that the steady state value of  $f(t)$  (which is the average volume fraction

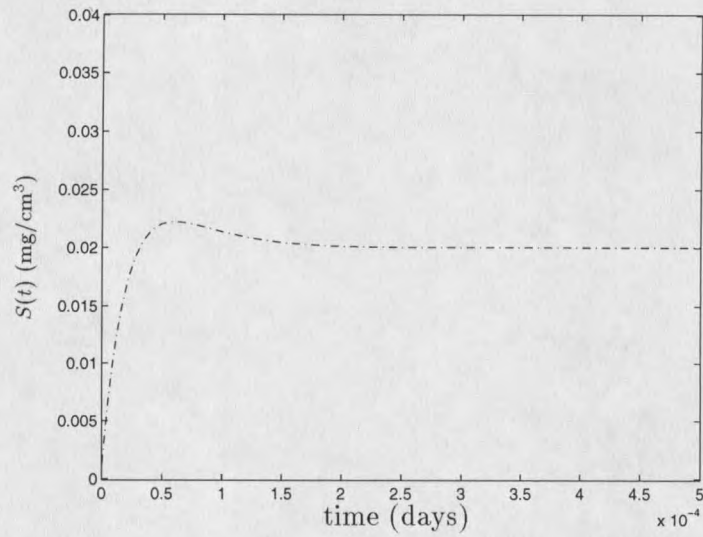


Figure 18: The substrate concentration,  $S(t)$ , over .0005 days for the zero-dimensional BGM

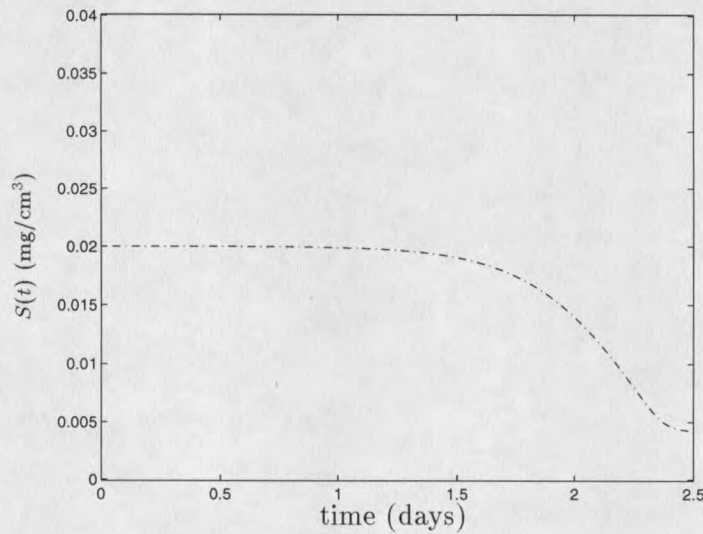


Figure 19: The substrate concentration,  $S(t)$ , over 2.5 days for the zero-dimensional BGM

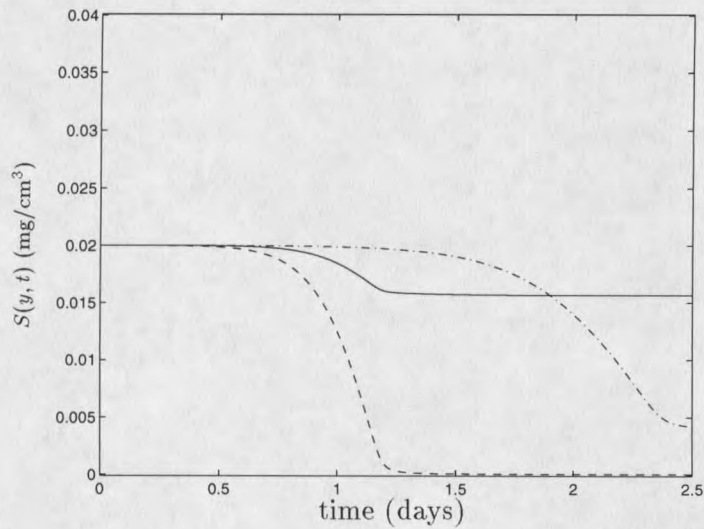


Figure 20: The substrate concentration,  $S(y, t)$ , at points  $y_1$  (dashed line) and  $y_2$  (solid line) in the biofilm over 2.5 days for the one-dimensional BGM and the substrate concentration,  $S(t)$ , (dash-dot line) over 2.5 days for the zero-dimensional BGM

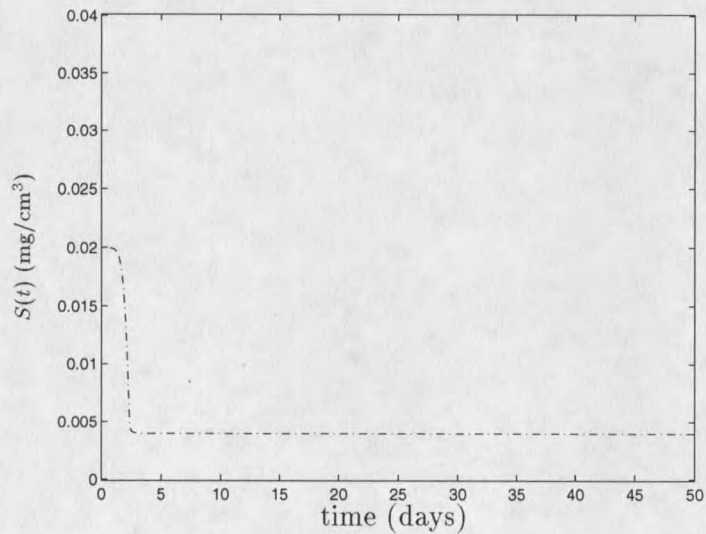


Figure 21: The substrate concentration,  $S(t)$ , over 50 days for the zero-dimensional BGM

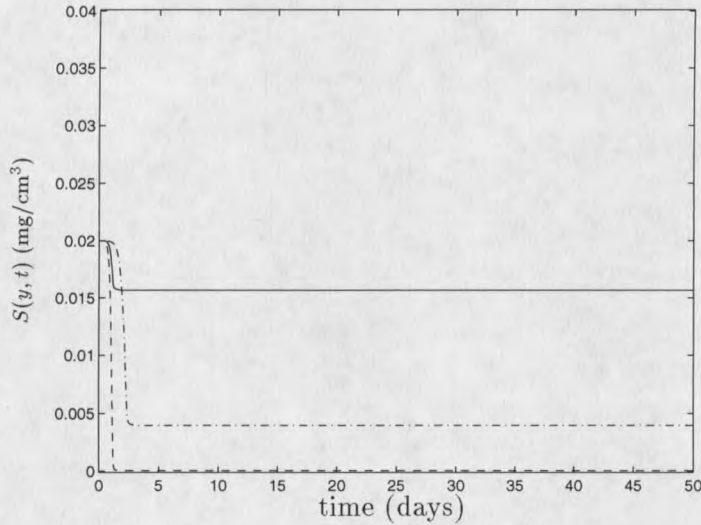


Figure 22: The substrate concentration,  $S(y, t)$ , at points  $y_1$  (dashed line ) and  $y_2$  (solid line) in the biofilm over 50 days for the one-dimensional BGM and the substrate concentration,  $S(t)$ , (dash-dot line) over 50 days for the zero-dimensional BGM

of active biomass) remains between the steady state values of  $f(y_1, t)$  and  $f(y_2, t)$  calculated from the one-dimensional BGM and the steady state value of  $\bar{f}(t)$  (which is the average volume fraction of inactive biomass) remains between the steady state values of  $\bar{f}(y_1, t)$  and  $\bar{f}(y_2, t)$  (see Figures 25 and 26). This shows a good agreement between the results of the zero-dimensional BGM and the one-dimensional BGM.

### Change in the Substrate Concentration in the Bulk Liquid

Figure 27 shows that the substrate concentration in the bulk liquid very quickly decreases from its initial value  $.04 \text{ mg/cm}^3$  to the influent substrate concentration,  $S_0 = .02 \text{ mg/cm}^3$ , and remains almost constant. A quantitative comparison of the numerical values of  $S_b$  from the one-dimensional and zero-dimensional models is given in Table 17. In this model we have assumed that the bulk liquid is constantly replaced by the substrate solution with constant substrate concentration,  $S_0 = .02 \text{ mg/cm}^3$ .

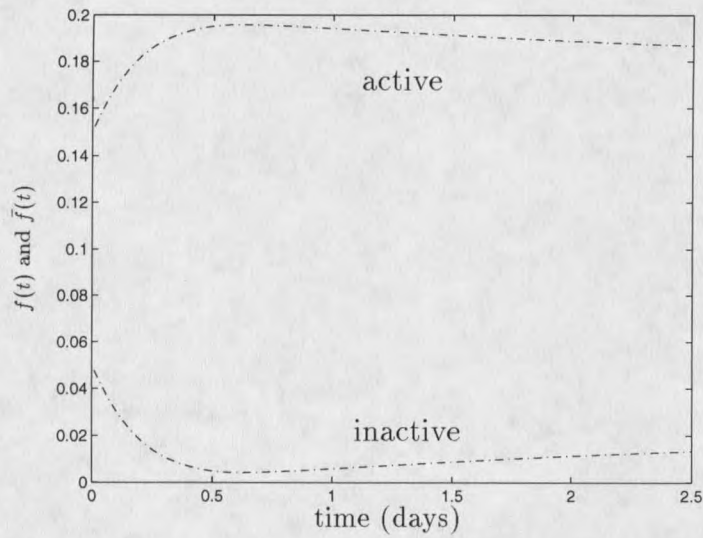


Figure 23: The active biomass volume fraction,  $f(t)$ , and inactive biomass volume fraction,  $\bar{f}(t)$ , over 2.5 days for the zero-dimensional BGM

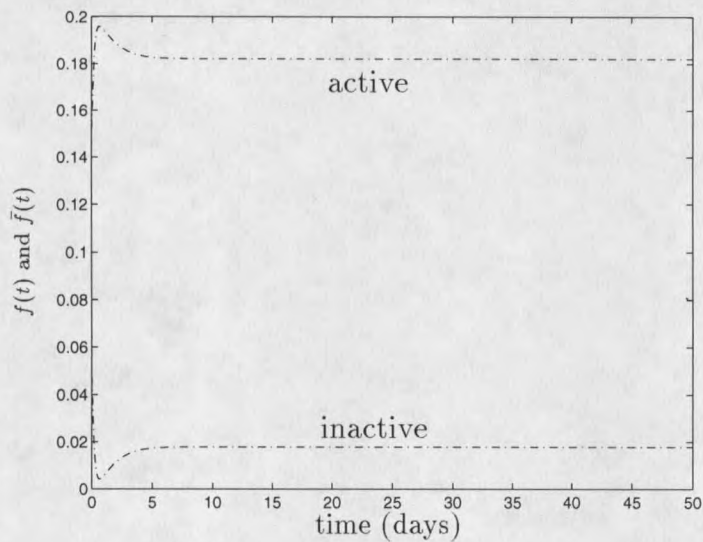


Figure 24: The active biomass volume fraction,  $f(t)$ , and inactive biomass volume fraction,  $\bar{f}(t)$ , over 50 days for the zero-dimensional BGM

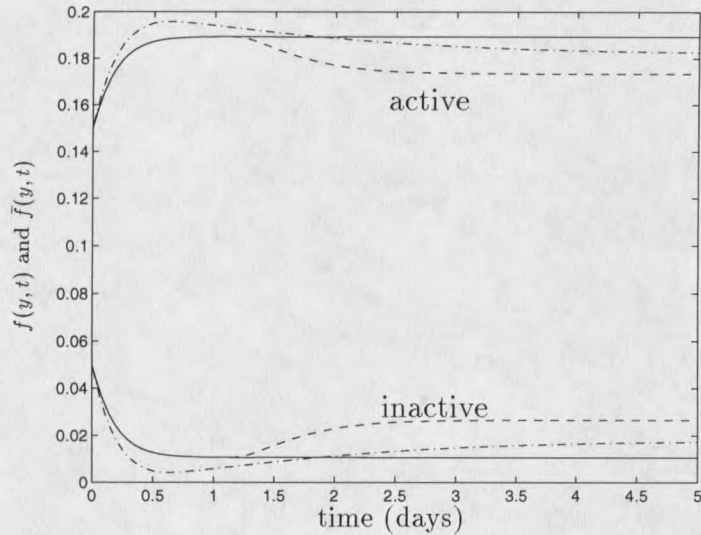


Figure 25: The active biomass volume fraction,  $f(t)$ , and inactive biomass volume fraction,  $\bar{f}(t)$ , over 5 days for the zero-dimensional BGM (dash-dot line) and the active biomass volume fraction,  $f(y, t)$ , and the inactive biomass volume fraction,  $\bar{f}(y, t)$ , at points  $y_1$  (dashed line) and  $y_2$  (solid line) over 5 days for the one-dimensional BGM

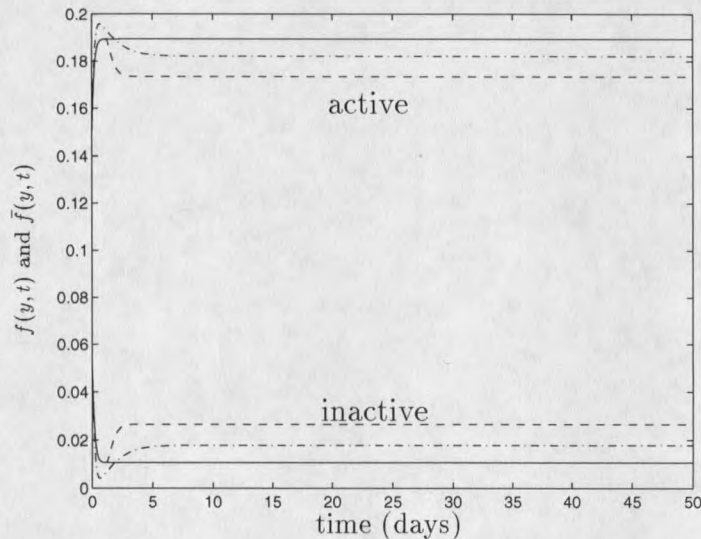


Figure 26: The active biomass volume fraction,  $f(t)$ , and inactive biomass volume fraction,  $\bar{f}(t)$ , over 50 days for the zero-dimensional BGM (dash-dot line) and the active biomass volume fraction,  $f(y, t)$ , and the inactive biomass volume fraction,  $\bar{f}(y, t)$ , at points  $y_1$  (dashed line) and  $y_2$  (solid line) over 50 days for the one-dimensional BGM

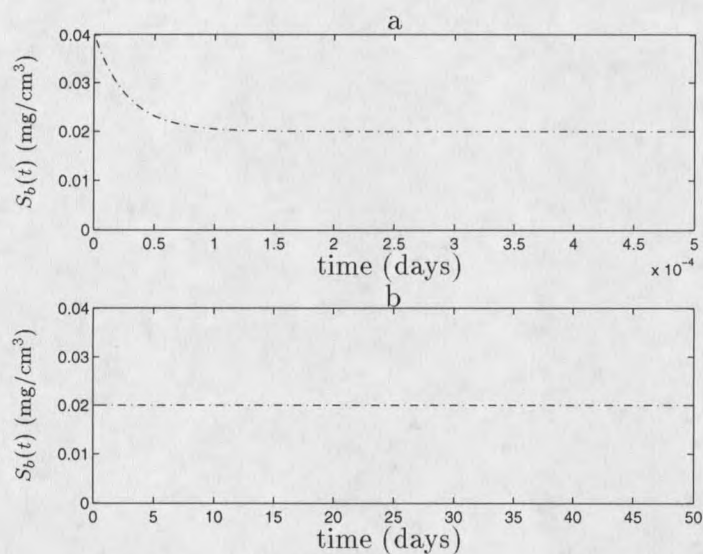


Figure 27: The substrate concentration,  $S_b(t)$ , in the bulk liquid, over .0005 days (a) and 50 days (b) for the zero-dimensional BGM

$t(\text{days})$	0-D $L(t)$ (cm)	1-D $L(t)$ (cm)
0.0	0.00005000	0.00005000
1.0	0.00393395	0.00308647
2.0	0.00712767	0.00819558
3.0	0.00796676	0.00820523
4.0	0.00812581	0.00820161
5.0	0.00814681	0.00820157
6.0	0.00814919	0.00820155
7.0	0.00815038	0.00820155
8.0	0.00815157	0.00820155
9.0	0.00815159	0.00820156
10.0	0.00815159	0.00820156
50.0	0.00815159	0.00820156

Table 11: Biofilm thickness,  $L(t)$ , over 50 days for the zero-dimensional and one-dimensional BGM

$t$ (days)	0-D $V_L(t)$ (cm <sup>3</sup> )	1-D $V_L(t)$ (cm <sup>3</sup> )
0.0	0.03000000	0.03000000
1.0	0.02611604	0.02696352
2.0	0.02292232	0.02185441
3.0	0.02208323	0.02184476
4.0	0.02192418	0.02184838
5.0	0.02190318	0.02184842
6.0	0.02190139	0.02184844
7.0	0.02189961	0.02184844
8.0	0.02189959	0.02184844
9.0	0.02189840	0.02184843
10.0	0.02189840	0.02184843
50.0	0.02189841	0.02184843

Table 12: Volume,  $V_L(t)$ , of the bulk liquid over 50 days for zero-dimensional and one-dimensional BGM

$t$ (days)	0-D $S(t)$ (mg/cm <sup>3</sup> )	1-D $S(y_1, t)$ (mg/cm <sup>3</sup> )	1-D $S(y_2, t)$ (mg/cm <sup>3</sup> )
0.00	0.00004000	0.00004000	0.00004000
0.20	0.01999329	0.01999163	0.01999826
0.40	0.01995124	0.01993918	0.01998741
0.60	0.01970063	0.01962661	0.01992272
0.80	0.01834961	0.01794149	0.01957394
1.00	0.01357709	0.01198887	0.01834175
1.20	0.00465585	0.00086576	0.01602612
1.40	0.00402774	0.00011370	0.01576986
1.60	0.00398152	0.00007518	0.01570053
1.80	0.00396847	0.00006677	0.01567356
2.00	0.00396329	0.00006412	0.01566080

Table 13: Substrate concentration,  $S(t)$ , in the biofilm for the zero-dimensional BGM and the substrate concentration,  $S(y, t)$ , at points  $y_1$  and  $y_2$  in the biofilm for the one-dimensional BGM over 2 days

$t$ (days)	0-D $S(t)$ (mg/cm <sup>3</sup> )	1-D $S(y_1, t)$ (mg/cm <sup>3</sup> )	1-D $S(y_2, t)$ (mg/cm <sup>3</sup> )
0.00	0.00004000	0.00004000	0.00004000
1.00	0.01357709	0.01198887	0.01834175
2.00	0.00396329	0.00006412	0.01566080
3.00	0.00396450	0.00006557	0.01566129
4.00	0.00396471	0.00006573	0.01566164
5.00	0.00396473	0.00006575	0.01566169
6.00	0.00396474	0.00006575	0.01566169
7.00	0.00396474	0.00006575	0.01566169
8.00	0.00396474	0.00006575	0.01566169
9.00	0.00396474	0.00006575	0.01566169
10.00	0.00396474	0.00006575	0.01566169
50.00	0.00396474	0.00006575	0.01566169

Table 14: Substrate concentration,  $S(t)$ , in the biofilm for the zero-dimensional BGM and the substrate concentration,  $S(y, t)$ , at points  $y_1$  and  $y_2$  in the biofilm for the one-dimensional BGM over 50 days

### Solution of Zero-dimensional Rittman's Model

The system of ordinary differential equations (2.39)-(2.42) is first simplified and then is solved using the code 'ODE23s' from MATLAB (version 4.2a). The computer code which approximates the solution of the zero-dimensional Rittman's model equations is given in Appendix D. Starting with (2.39)

$$\frac{dS_b(t)}{dt} = \frac{1}{V_L} \left( QS_0 - \left( Q + \frac{\sigma D}{L_l} \right) S_b(t) + \frac{\sigma D}{L_l} S(t) \right),$$

we write this as

$$\frac{dS_b(t)}{dt} = \frac{1}{V_L} \left( QS_0 - QS_b(t) - \frac{\sigma D}{L_l} S_b(t) + \frac{\sigma D}{L_l} S(t) \right). \quad (3.12)$$

Similarly (2.42) is written

$$\frac{dL(t)}{dt} = \left( \left( Y \frac{V_r S(t)}{K + S(t)} - bf_d \right) f(t) - B' \right) L(t). \quad (3.13)$$

$t$ (days)	0-D $f(t)$	1-D $f(y_1, t)$	1-D $f(y_2, t)$
0.00	0.15000000	0.15000000	0.15000000
0.50	0.19520130	0.18733056	0.18733068
1.00	0.19424553	0.18932086	0.18933049
1.50	0.19115583	0.18401590	0.18931887
2.00	0.18869909	0.17633567	0.18933877
2.50	0.18688385	0.17421025	0.18940333
3.10	0.18506860	0.17357378	0.18940975
3.50	0.18406933	0.17348751	0.18940770
4.00	0.18357616	0.17347671	0.18940714
4.50	0.18308299	0.17346572	0.18940654
5.00	0.18261836	0.17346543	0.18940649
10.30	0.18212676	0.17346527	0.18940646
15.30	0.18212592	0.17346525	0.18940646
20.30	0.18212610	0.17346525	0.18940646
25.30	0.18212607	0.17346525	0.18940646
30.30	0.18212607	0.17346525	0.18940646
35.30	0.18212607	0.17346525	0.18940646

Table 15: Active biomass volume fraction,  $f(t)$ , for the zero-dimensional BGM and active biomass volume fraction,  $f(y, t)$ , at points  $y_1$  and  $y_2$  in the biofilm for the one-dimensional BGM over 35 days

$t$ (days)	0-D $\bar{f}(t)$	1-D $\bar{f}(y_1, t)$	1-D $\bar{f}(y_2, t)$
0.00	0.05000000	0.05000000	0.05000000
0.50	0.00479869	0.01266943	0.01266931
1.00	0.00575446	0.01067913	0.01066950
1.50	0.00884416	0.01598409	0.01068112
2.00	0.01130090	0.02366432	0.01066122
2.50	0.01311614	0.02578974	0.01059666
3.00	0.01493139	0.02642621	0.01059024
3.50	0.01593066	0.02651248	0.01059229
4.00	0.01642383	0.02652328	0.01059285
4.50	0.01691700	0.02653427	0.01059345
5.00	0.01738163	0.02653456	0.01059350
10.00	0.01787323	0.02653472	0.01059353
15.00	0.01787407	0.02653474	0.01059353
20.00	0.01787389	0.02653474	0.01059353
25.00	0.01787392	0.02653474	0.01059353
30.00	0.01787392	0.02653474	0.01059353
35.30	0.01787392	0.02653474	0.01059353

Table 16: Inactive biomass volume fraction,  $\bar{f}(t)$ , for the zero-dimensional BGM and inactive biomass volume fraction,  $\bar{f}(y, t)$ , at points  $y_1$  and  $y_2$  in the biofilm for the one-dimensional BGM over 35 days

$t$ (days)	0-D $S_b(t)$ (mg/cm <sup>3</sup> )	1-D $S_b(t)$ (mg/cm <sup>3</sup> )
0.000000	0.04000000	0.04000000
0.000020	0.02980148	0.02942642
0.000040	0.02433157	0.02451977
0.000060	0.02224666	0.02213547
0.000080	0.02090228	0.02108512
0.000100	0.02047238	0.02057680
0.000120	0.02020717	0.02026683
0.000140	0.02010431	0.02009900
0.000160	0.02005596	0.02006178
0.000180	0.02001375	0.02002456
0.000200	0.02001274	0.02001333
0.000400	0.01999888	0.01999984
0.000600	0.01999889	0.02000004
0.000800	0.01999889	0.02000003
0.001000	0.01999888	0.02000002

Table 17: The bulk substrate concentration,  $S_b(t)$ , for the zero-dimensional and one-dimensional BGM over .001 days

Next (2.40)

$$\frac{d}{dt} \left( L(t)S(t) \right) = \frac{D}{L_l} \left( S_b(t) - S(t) \right) - \frac{V_r S(t)}{K + S(t)} L(t) f(t) \rho$$

is written as

$$\frac{dS(t)}{dt} = \left( -\frac{S(t)}{L(t)} \frac{dL(t)}{dt} + \frac{D}{L(t)L_l} (S_b(t) - S(t)) - \frac{V_r S(t)}{K + S(t)} f(t) \rho \right).$$

Using (3.13) this becomes

$$\begin{aligned} \frac{dS(t)}{dt} = & \left( -\left( Y \frac{V_r S(t)}{K + S(t)} - b f_d \right) f(t) + B' \right) S(t) \\ & + \frac{D}{L(t)L_l} (S_b(t) - S(t)) - \frac{V_r S(t)}{K + S(t)} f(t) \rho \end{aligned}$$

which reduces to

$$\frac{dS(t)}{dt} = -\frac{V_r f(t) S(t)}{K + S(t)} \left( Y S(t) + \rho \right) + b f_d f(t) S(t) + B' S(t)$$

$$+\frac{D}{L(t)L_i} \left( S_b(t) - S(t) \right). \quad (3.14)$$

Finally, (2.41)

$$\frac{d}{dt} \left( L(t)f(t) \right) = \left( Y \frac{V_r S(t)}{K + S(t)} - (b + B') \right) L(t)f(t)$$

becomes

$$\frac{df(t)}{dt} = -\frac{f(t)}{L(t)} \frac{dL(t)}{dt} + Y \frac{V_r S(t)f(t)}{K + S(t)} - (b + B')f(t).$$

Again using (3.13) this reduces to

$$\begin{aligned} \frac{df(t)}{dt} = & - \left( Y \frac{V_r S(t)}{K + S(t)} - b f_d \right) f^2(t) + B' f(t) \\ & + \frac{Y V_r S(t)f(t)}{K + S(t)} - (b + B')f(t) \end{aligned}$$

which simplifies to

$$\frac{df(t)}{dt} = \left( \frac{Y V_r S(t)}{K + S(t)} (1 - f(t)) - b(1 - f_d f(t)) \right) f(t). \quad (3.15)$$

The system of equations (3.12)-(3.15) is solved using the parameter values and the initial values given in Table 18. The system is solved for four unknown variables; substrate concentration in the bulk liquid,  $S_b(t)$ , thickness of the biofilm,  $L(t)$ , the average substrate concentration in the biofilm,  $S(t)$ , and the average volume fraction of the biomass in the biofilm,  $f(t)$ .

A qualitative analysis of the numerical results is given in Figures 28 through 31. Figure 28 contains the graphs of  $S_b(t)$  and  $S(t)$  as functions of time,  $t$ . Each of the figures (Figures 29-31) contains the graphs of  $S_b(t)$ ,  $L(t)$ ,  $S(t)$ , and  $f(t)$  as functions of time,  $t$ .

Since the volumetric flow rate is relatively high, the substrate concentration in the bulk liquid very quickly (within .01 days) decreases to the influent substrate concentration,  $S_0 = .02 \text{ mg/cm}^3$ , as seen in Figure 28. The substrate concentration in

Parameters	Values	Units
$K$	0.0001	mg/cm <sup>3</sup>
$V_r$	4.3	mg/(mg day)
$Y$	.2	mg/mg
$b$	.35	day <sup>-1</sup>
$D$	1.3	cm <sup>2</sup> /day
$V_L$	2.0	cm <sup>3</sup>
$Q$	1100	cm <sup>3</sup> /day
$\sigma$	1	cm <sup>2</sup>
$L_l$	.8	cm
$\rho$	12.2	mg/cm <sup>3</sup>
$B'$	.31	day <sup>-1</sup>
$S_0$	.02	mg/cm <sup>3</sup>
$f_d$	0	dimensionless
Variables	Initial Values	Units
$S_b(0)$	.04	mg/cm <sup>3</sup>
$L(0)$	.00005	cm
$S(0)$	.00004	mg/cm <sup>3</sup>
$f(0)$	.2	dimensionless

Table 18: Parameter values and initial values for the zero-dimensional Rittman's model

the biofilm,  $S(t)$ , rises initially (for the first .0002 days) because of the high concentration difference across the interface. After .0002 days (17.3 sec)  $S_b(t)$  and  $S(t)$  have the same value (around .038 mg/cm<sup>3</sup>). Since the substrate concentration difference across the film-water interface is zero there (at  $t = .0002$  days),  $S(t)$  stops increasing which can be visualized in Figure 28 as the slope of  $S(t)$  is zero at  $t = .0002$  days. The two substrate concentrations  $S_b(t)$  and  $S(t)$  decrease to the influent substrate concentration,  $S_0 = .02$  mg/cm<sup>3</sup> within .01 days. As the consumption of the substrate becomes significant,  $S(t)$  begins to decrease (see Figure 30c). The active bacteria in the biofilm consume the substrate and multiply which causes a rapid increase in the volume fraction of the active biomass,  $f(t)$  which can be seen in Figure 30d. As long as  $S(t)$  is sufficiently high (close to .02 mg/cm<sup>3</sup>),  $f(t)$  increases rapidly. Between the sixth and the twelfth days, the biofilm thickness increases rapidly causing a rapid decrease in  $S(t)$ . The decay in  $S(t)$  controls the growth of  $L(t)$  and  $f(t)$ . All the variables reach their steady states after 30 days (see Figure 31).

### Solution of Zero-dimensional BAM

The system of ordinary differential equations (2.76) - (2.79) is first simplified and then is solved using the code 'ODE23s' from MATLAB (version 4.2a). The computer code which approximates the solution of the zero-dimensional BAM equations is given in Appendix E. Beginning with (2.76)

$$\frac{dL(t)}{dt} = \frac{1}{1 - \epsilon_l} \frac{Y R(t) L(t)}{\rho} + \delta(t). \quad (3.16)$$

Next is (2.77)

$$\frac{d}{dt} (L(t) f(t)) = \frac{Y R(t) L(t)}{\rho} - b L(t) f(t) + \delta(t) f(t).$$

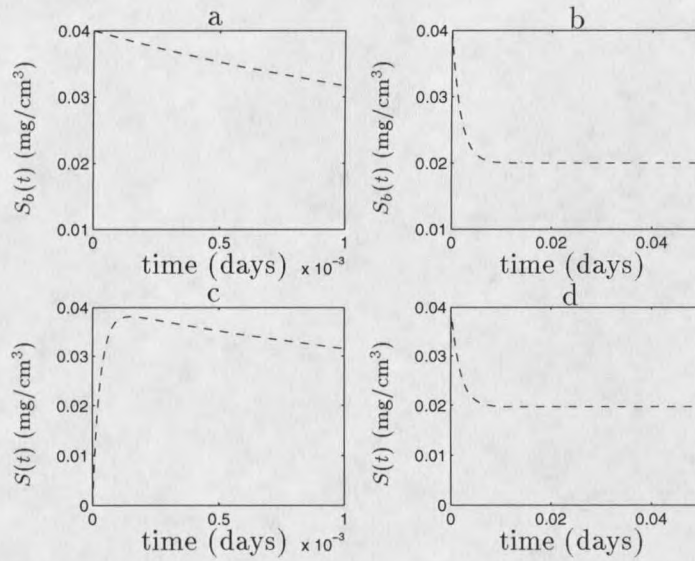


Figure 28: Bulk substrate concentration,  $S_b(t)$  over .001 days, (a), and .05 days, (b) and substrate concentration in the biofilm,  $S(t)$ , over .001 days, (c), and .05 days, (d) for the zero-dimensional Rittman's model

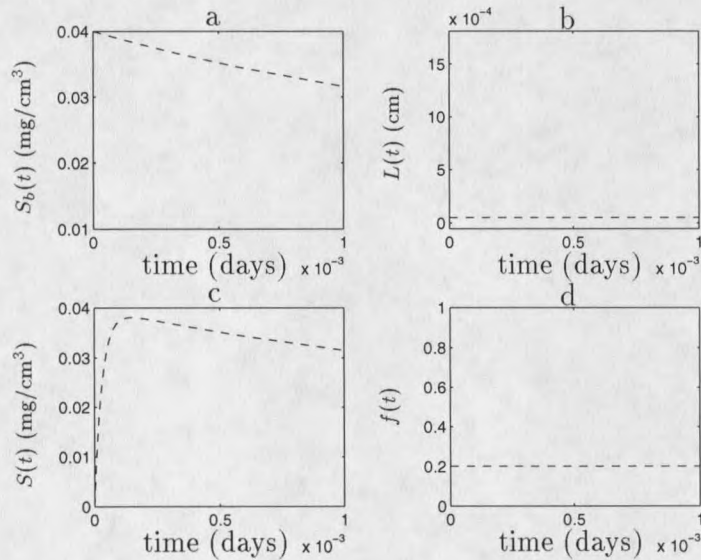


Figure 29: Bulk substrate concentration,  $S_b(t)$ , (a), biofilm thickness,  $L(t)$ , (b), substrate concentration in the biofilm,  $S(t)$ , (c), and active biomass volume fraction,  $f(t)$ , (d), over .001 days for the zero-dimensional Rittman's model

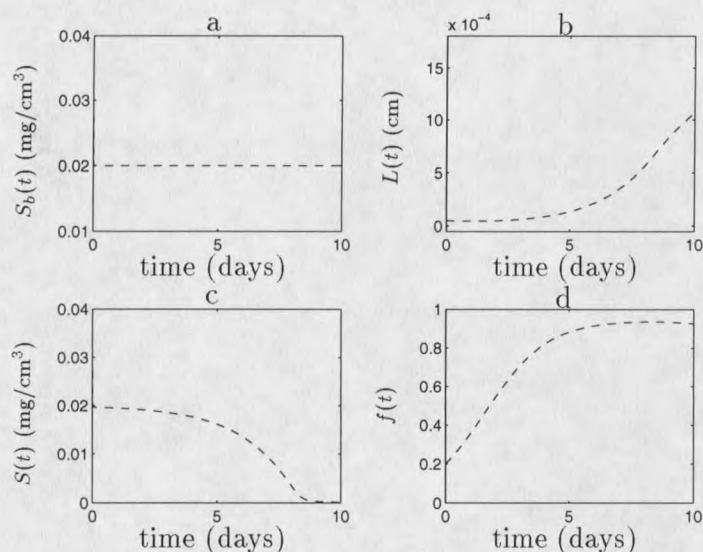


Figure 30: Bulk substrate concentration,  $S_b(t)$ , (a), biofilm thickness,  $L(t)$ , (b), substrate concentration in the biofilm,  $S(t)$ , (c), and active biomass volume fraction,  $f(t)$ , (d), over 10 days for the zero-dimensional Rittman's model

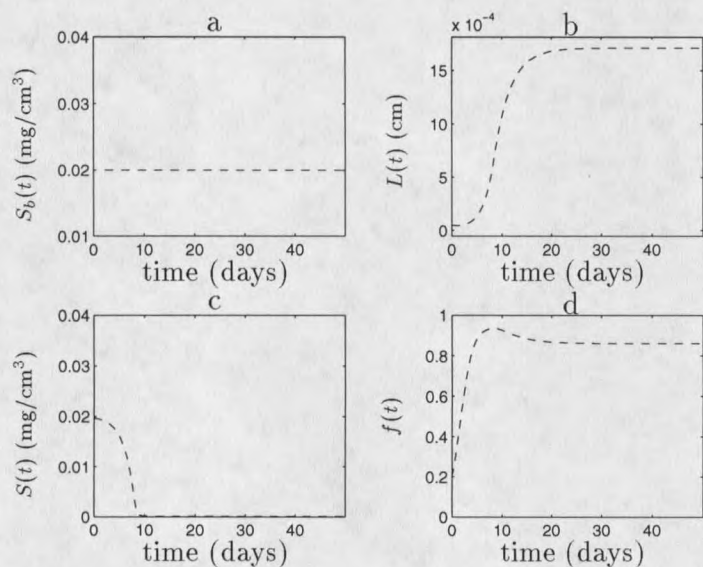


Figure 31: Bulk substrate concentration,  $S_b(t)$ , (a), biofilm thickness,  $L(t)$ , (b), substrate concentration in the biofilm,  $S(t)$ , (c), and active biomass volume fraction,  $f(t)$ , (d), over 50 days for the zero-dimensional Rittman's model

Using the chain rule and (3.16) this reduces to

$$\frac{df(t)}{dt} = -\frac{f(t)}{L(t)} \left( \frac{1}{1-\epsilon_l} \frac{YR(t)L(t)}{\rho} + \delta(t) \right) + \frac{YR(t)}{\rho} - bf(t) + \frac{\delta(t)f(t)}{L(t)}$$

which simplifies to

$$\frac{df(t)}{dt} = \frac{YR(t)}{\rho} \left( 1 - \frac{f(t)}{1-\epsilon_l} \right) - bf(t). \quad (3.17)$$

Similarly (2.78)

$$\frac{d}{dt} \left( L(t)S(t) \right) = \frac{D}{L_l} \left( S_b(t) - S(t) \right) - R(t)L(t)$$

reduces to

$$\frac{dS(t)}{dt} = -\frac{S(t)}{L(t)} \left( \frac{1}{1-\epsilon_l} \frac{YR(t)L(t)}{\rho} + \delta(t) \right) + \frac{D}{L_l L(t)} \left( S_b(t) - S(t) \right) - R(t)$$

which further simplifies to

$$\begin{aligned} \frac{dS(t)}{dt} &= -\frac{R(t)}{\rho} \left( \rho + \frac{YS(t)}{1-\epsilon_l} \right) - \frac{\delta(t)S(t)}{L(t)} \\ &\quad + \frac{D}{L_l L(t)} (S_b(t) - S(t)). \end{aligned} \quad (3.18)$$

Lastly (2.79)

$$\begin{aligned} \frac{dS_b(t)}{dt} &= \frac{1}{V_L} \left[ Q \left( S_0 - S_b(t) \right) - \sigma \left( \frac{D}{L_l} - u_L(t) \right) \right. \\ &\quad \left. \left( S_b(t) - S(t) \right) \right] \end{aligned}$$

becomes

$$\begin{aligned} \frac{dS_b(t)}{dt} &= \frac{1}{V_L} \left[ Q \left( S_0 - S_b(t) \right) - \sigma \left\{ \frac{D}{L_l} - \left( \frac{1}{1-\epsilon_l} \frac{YR(t)L(t)}{\rho} + \delta(t) \right) \right\} \right. \\ &\quad \left. \left( S_b(t) - S(t) \right) \right]. \end{aligned} \quad (3.19)$$

By [25], appropriate choices for  $R(t)$  and  $\delta(t)$  are

$$R(t) = \frac{V_r S(t) \rho f(t)}{K + S(t)} \quad (3.20)$$

and

$$\delta(t) = -\lambda(L(t))^2. \quad (3.21)$$

This system is solved for four unknown variables; substrate in the bulk liquid,  $S_b(t)$ , thickness of the biofilm,  $L(t)$ , the average substrate concentration in the biofilm,  $S(t)$ , and the average volume fraction of the biomass in the biofilm,  $f(t)$ . The values of the parameters and the initial values of the variables are given in Table 19.

A qualitative analysis of the numerical results is given in Figures 32 through 35. Figure 32 contains the graphs of  $S_b(t)$  and  $S(t)$  as functions of time,  $t$ . Each of the figures (Figures 33-35) contains the graphs of  $S_b(t)$ ,  $L(t)$ ,  $S(t)$ , and  $f(t)$  as functions of time,  $t$ .

Parameters	Values	Units
$K$	0.0001	mg/cm <sup>3</sup>
$V_r$	4.3	mg/(mg day)
$Y$	.2	mg/mg
$b$	.35	day <sup>-1</sup>
$D$	1.3	cm <sup>2</sup> /day
$V_L$	2.0	cm <sup>3</sup>
$\epsilon_i$	0.0	dimensionless
$Q$	1100	cm <sup>3</sup> /day
$\sigma$	1	cm <sup>2</sup>
$L_l$	.8	cm
$\rho$	12.2	mg/cm <sup>3</sup>
$S_0$	.02	mg/cm <sup>3</sup>
$\lambda$	500	cm <sup>-1</sup> day <sup>-1</sup>
Variables	Initial Values	Units
$S_b(0)$	.04	mg/cm <sup>3</sup>
$L(0)$	.00005	cm
$S(0)$	.00004	mg/cm <sup>3</sup>
$f(0)$	.2	dimensionless

Table 19: Parameters values and the initial values for the zero-dimensional BAM

We begin the qualitative analysis of the change in dependents variables with the substrate concentration,  $S_b(t)$ . Figure 32 shows that  $S_b(t)$  very quickly (within

.01 days) decreases from its initial value  $S_b(0) = .04 \text{ mg/cm}^3$  to the constant substrate concentration  $S_0 = .02 \text{ mg/cm}^3$  which is the substrate concentration of the influent fluid. Figure 34a and Figure 35a show that the substrate concentration does not change with time because the influent fluid of constant substrate concentration continuously keeps replacing the old fluid. The substrate concentration in the biofilm,  $S(t)$ , rises initially (for the first .0002 days) because of the high concentration difference across the interface. After .0002 days (17.3 sec)  $S_b(t)$  and  $S(t)$  have the same value (around .038  $\text{mg/cm}^3$ ). Since the substrate concentration difference across the film-water interface is zero there (at  $t = .0002$  days),  $S(t)$  stops increasing which can be visualized in Figure 32 as the slope of  $S(t)$  is zero at  $t = .0002$  days. The two substrate concentrations  $S_b(t)$  and  $S(t)$  decrease to the influent substrate concentration,  $S_0 = .02 \text{ mg/cm}^3$  within .01 days. As the consumption of the substrate becomes significant,  $S(t)$  begins to decrease (see Figure 34c). The active bacteria in the biofilm consume the substrate and multiply which causes a rapid increase in the volume fraction of the active biomass,  $f(t)$  which can be seen in Figure 34d. As long as  $S(t)$  is sufficiently high (close to .02  $\text{mg/cm}^3$ ),  $f(t)$  increases rapidly. Between day 6 and day 12, the biofilm thickness increases rapidly causing a rapid decrease in  $S(t)$ . The decay in  $S(t)$  controls the growth of  $L(t)$  and  $f(t)$ . All the variables reach their steady states after 30 days (see Figure 35).









































































































































































































































































